

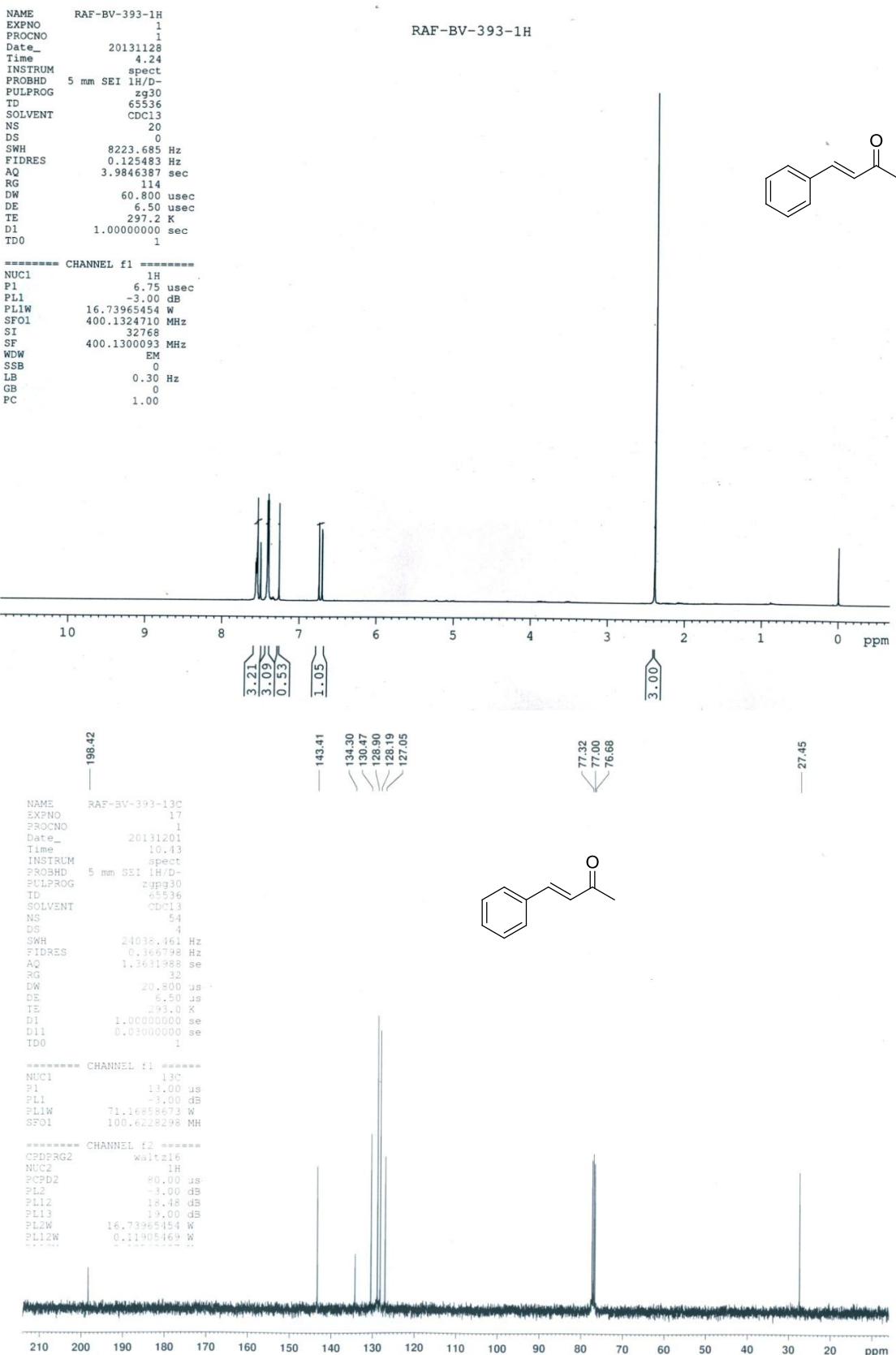
## Supporting Information

# **Traceless OH-directed Wacker Oxidation-Elimination, an Alternative to Wittig Olefination/Aldol Condensation: One-pot Synthesis of $\alpha,\beta$ -Unsaturated and Non-conjugated Ketones from Homoallyl Alcohols**

Venkati Bethi and Rodney A. Fernandes\*

$^1\text{H}$  and  $^{13}\text{C}$  NMR for **2a-2r**, **4a-4g** and **6a-6j** ----- S1-S36

**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 2a**



**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 2b**

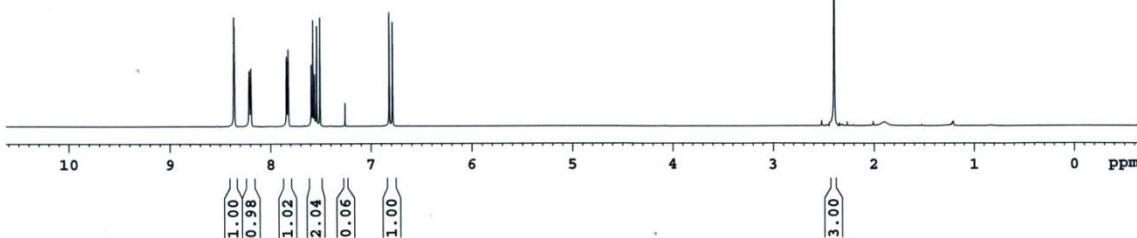
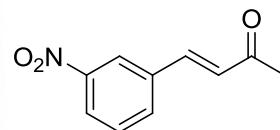
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EXPNO 1  
PROCNO 1

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Date 20150703  
Time 9.53  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 10  
DS 0  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.2767999 sec  
RG 37.72  
DW 50.00 usec  
DE 6.50 usec  
TE 296.2 K  
D1 1.0000000 sec  
TDO 1

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
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NUC1 1H  
P1 13.00 usec  
PLW1 13.00000000 W

F2 - Processing parameters  
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WDW EM  
SSB 0  
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PC 1.00

RAF-BV-GVR-6-761-1H



197.52

Current Data Parameters  
NAME RAF-BV-GVR-6-761-13C  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date 20150702  
Time 19.20  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpp30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 21  
DS 0  
SWH 29761.900 Hz  
FIDRES 0.454131 Hz  
AQ 1.101000 sec  
RG 1.97.27  
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TDO 1

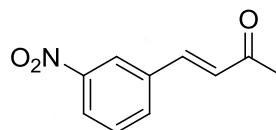
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\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
SP02 500.1320005 MHz  
NUC2 1H  
CPDPG[2] waltz16  
CPDPG2 80.00 usec  
PLW2 13.0000000 W  
PLW12 0.34327999 W  
PLW13 0.21369999 W

F2 - Processing parameters  
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WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

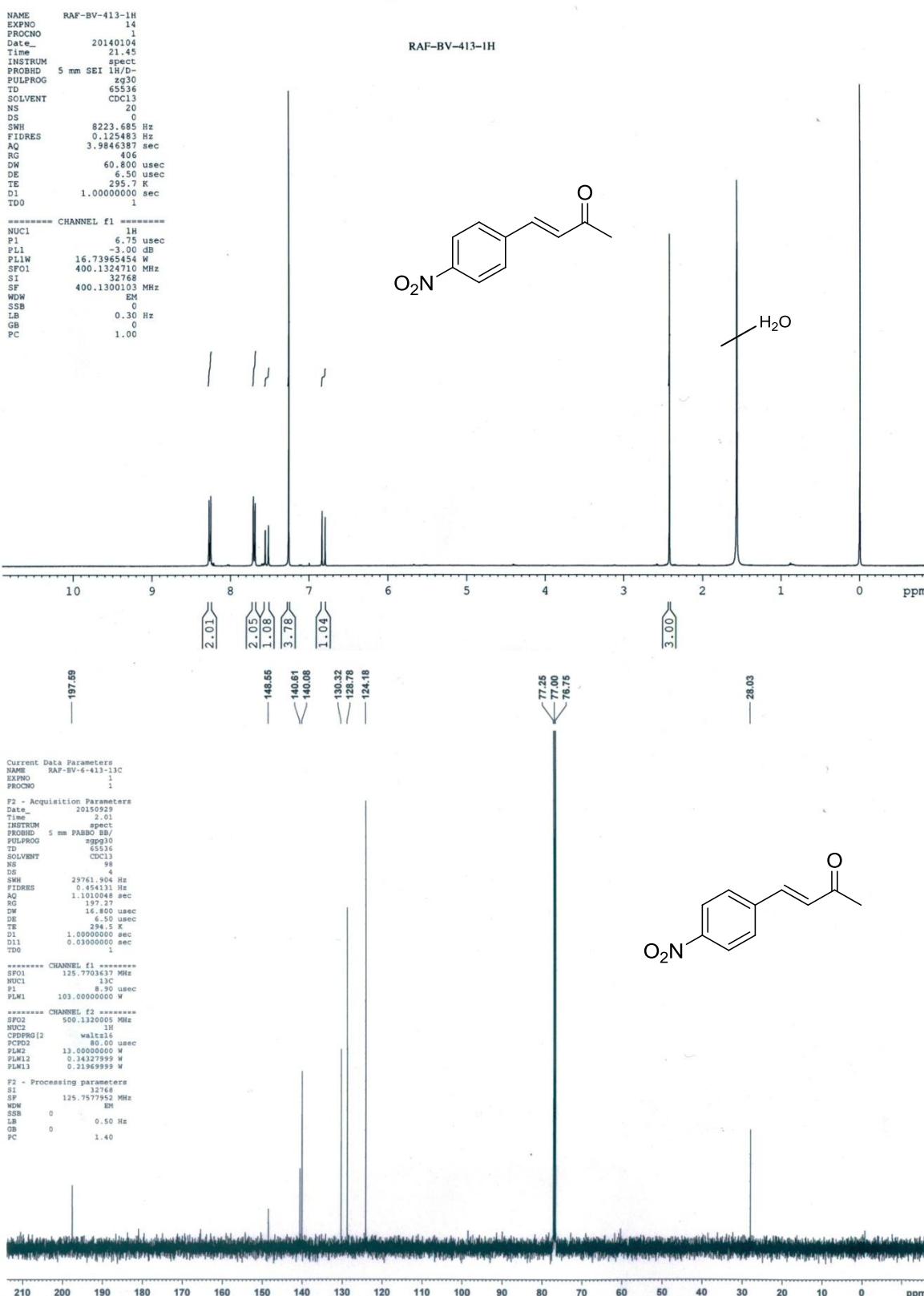
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27.93

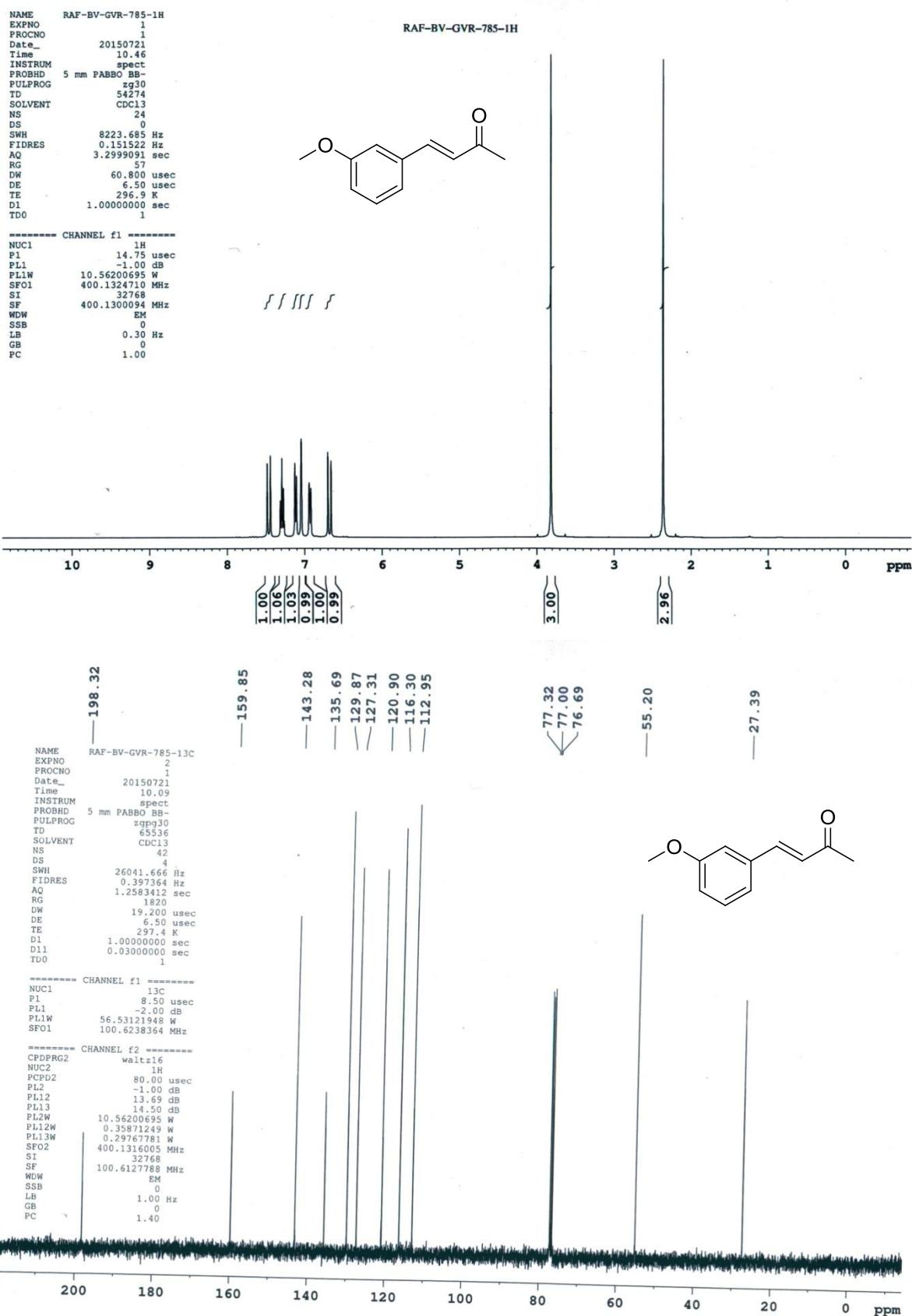


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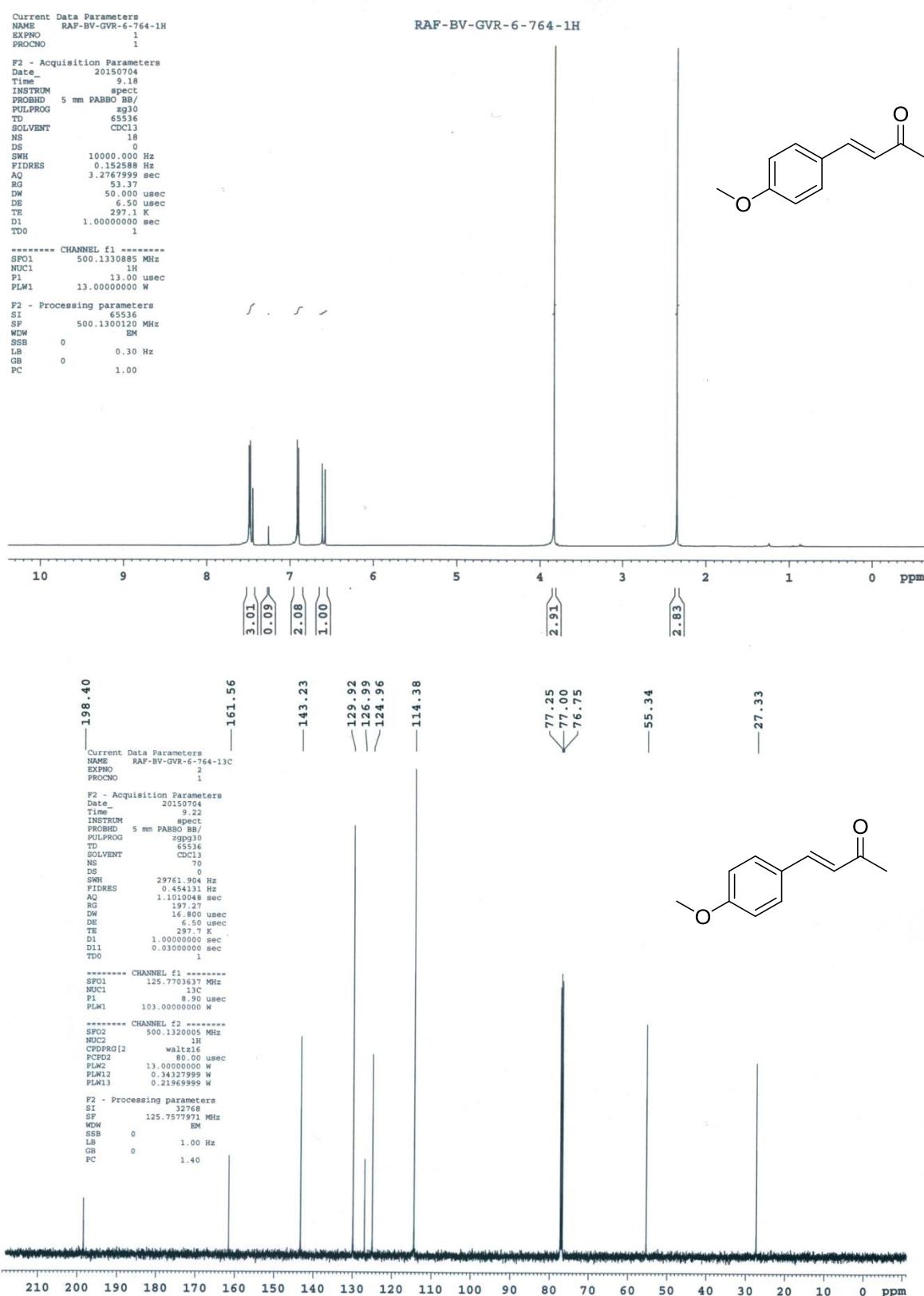
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 2c**



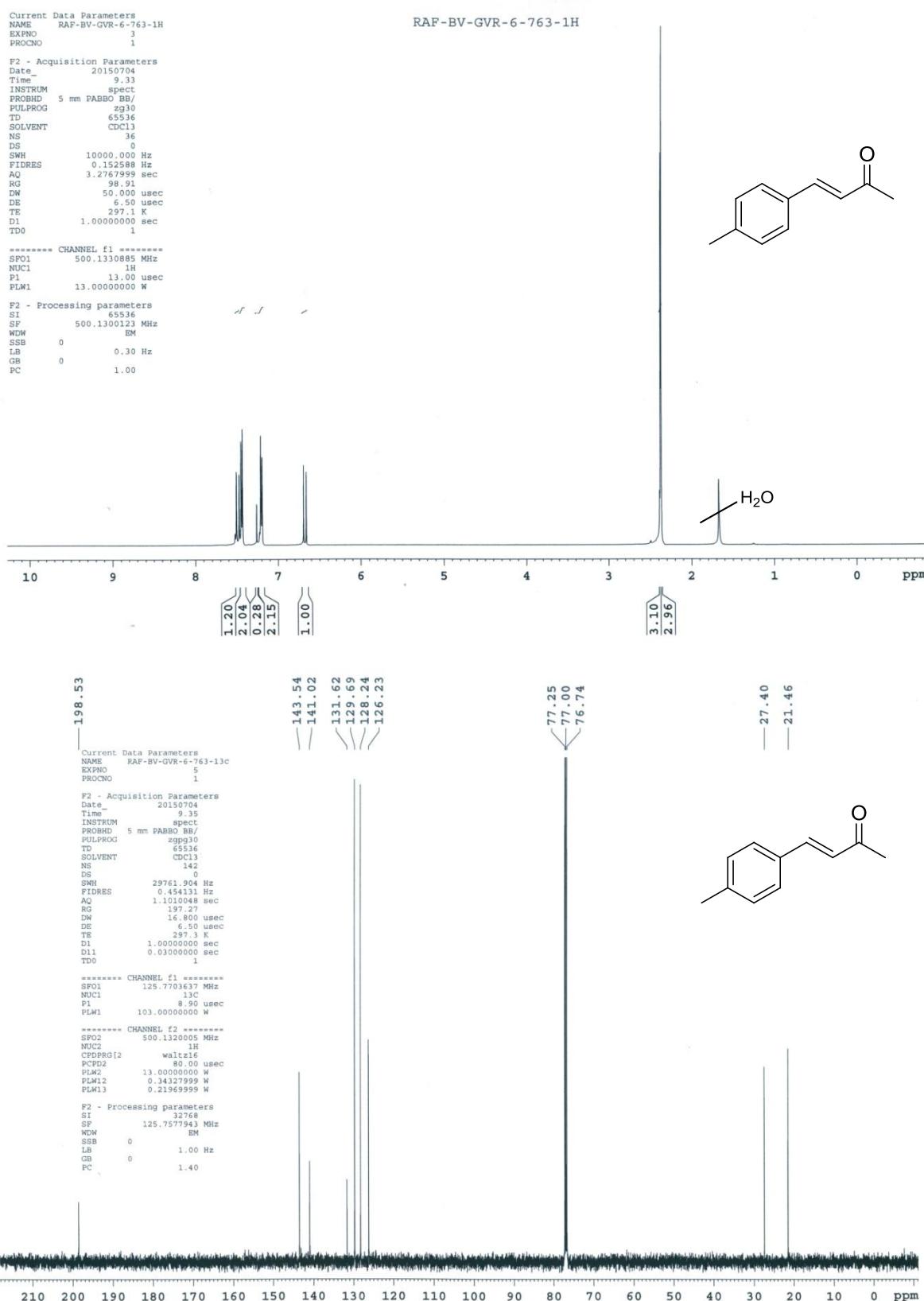
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 2d**



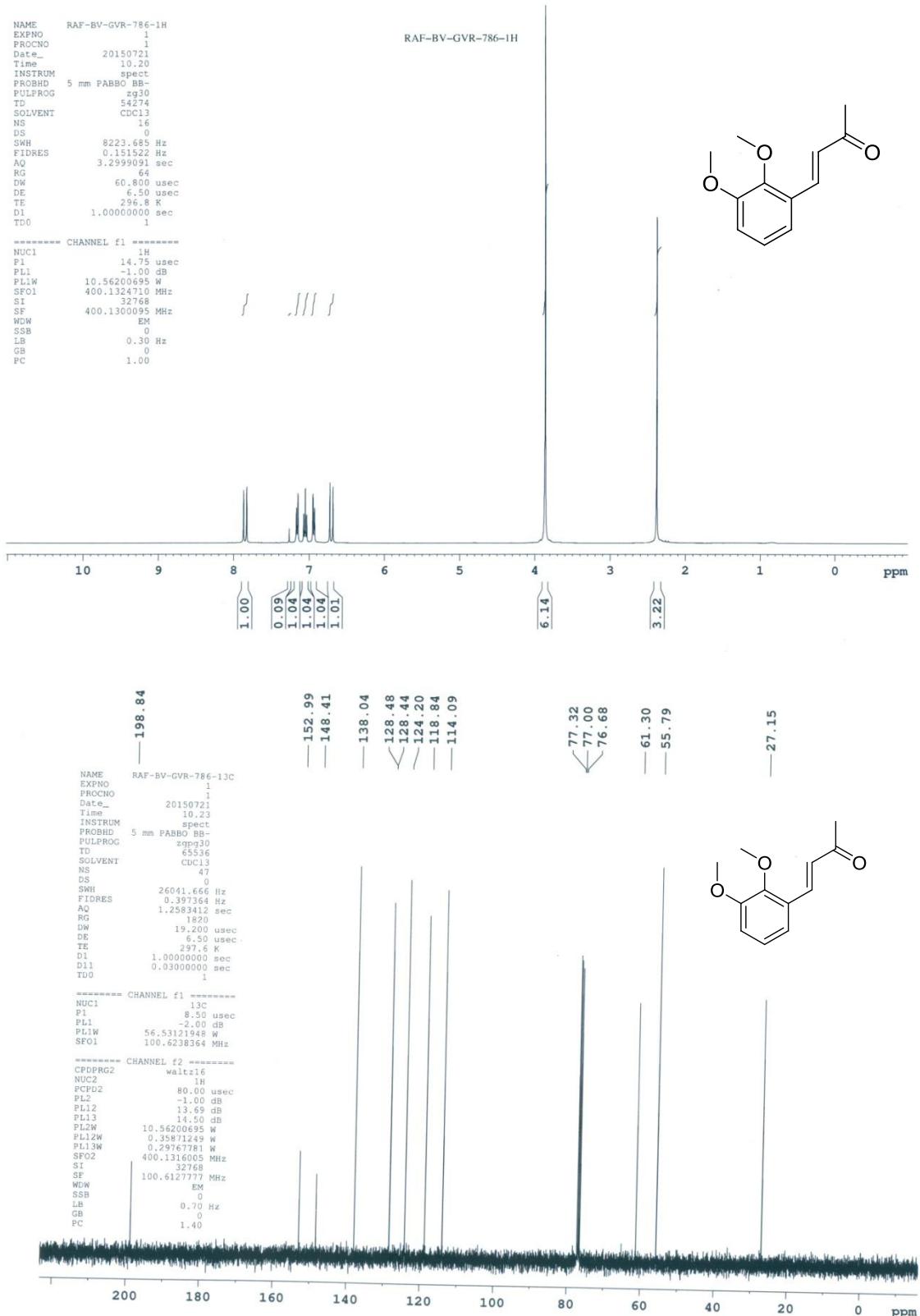
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 2e**



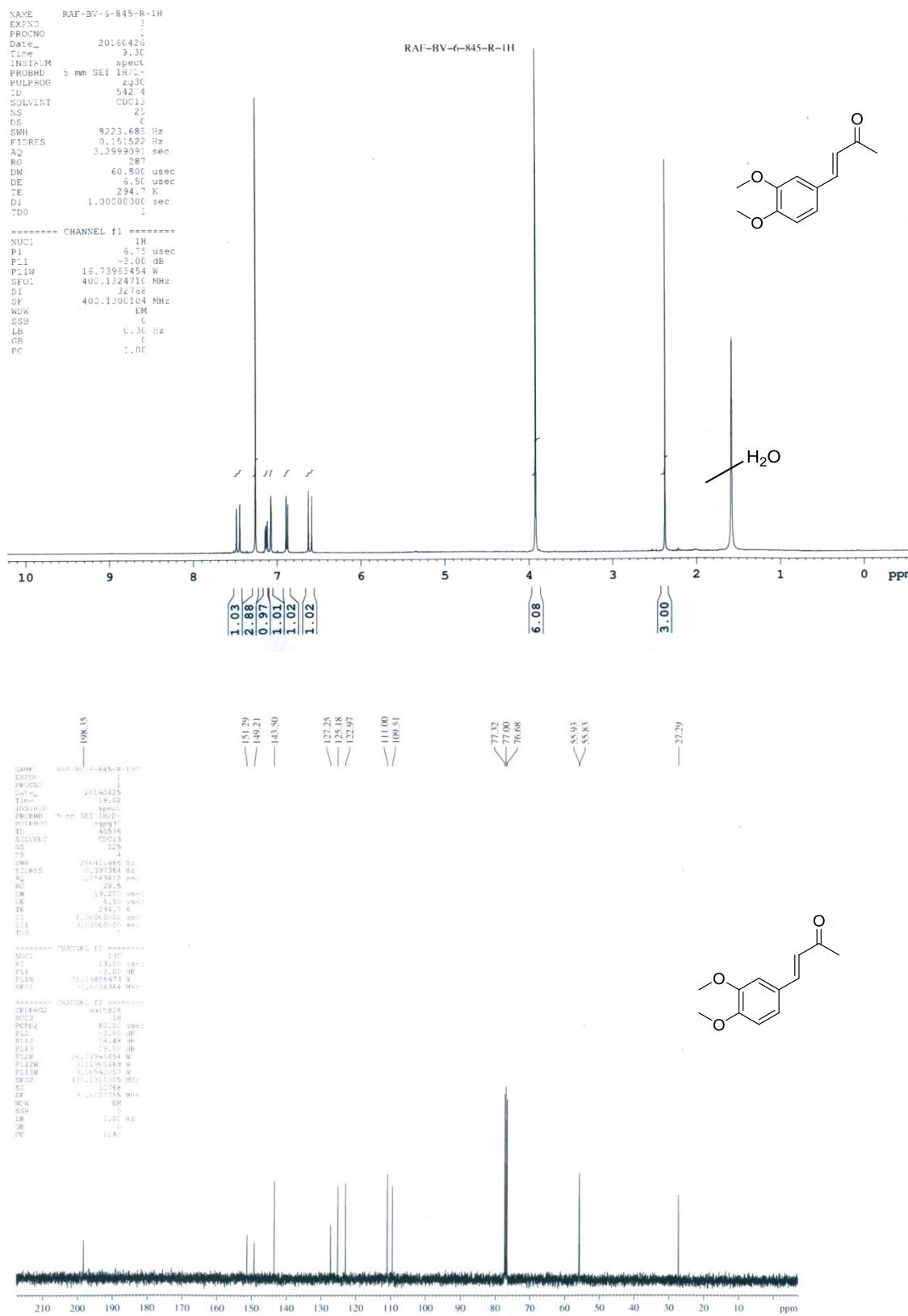
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 2f**



**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 2g**



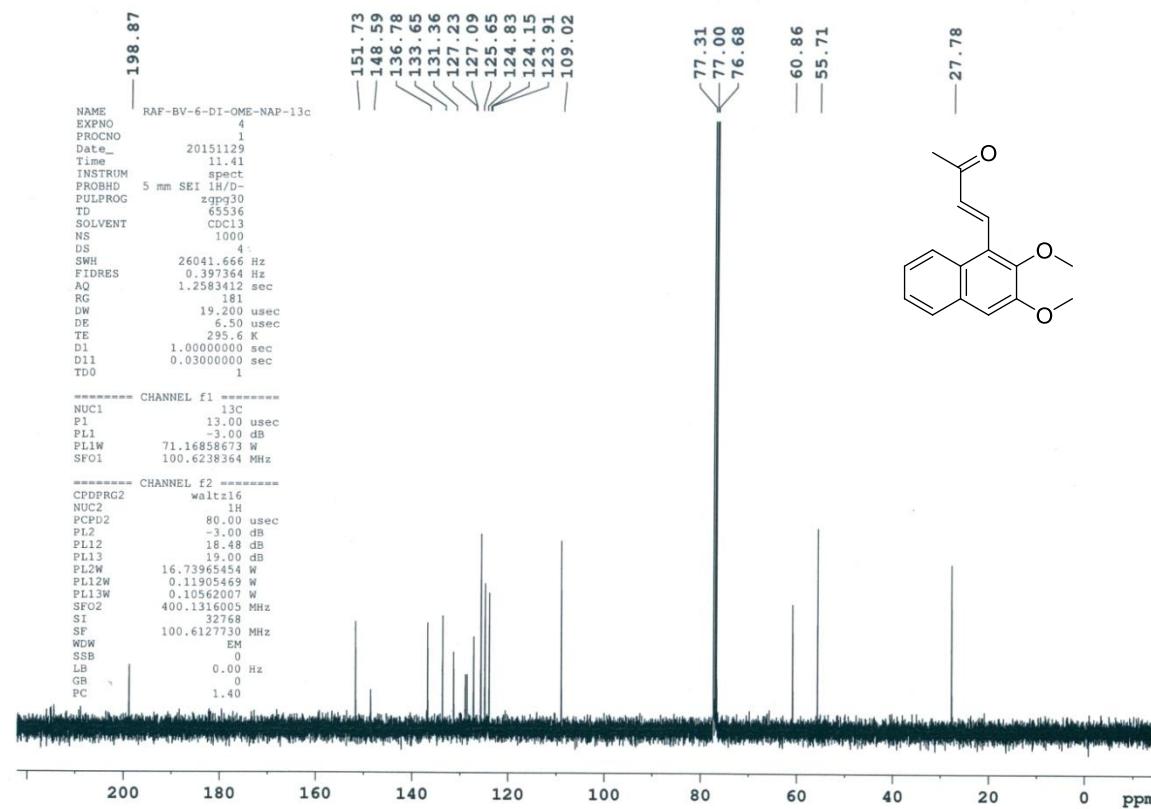
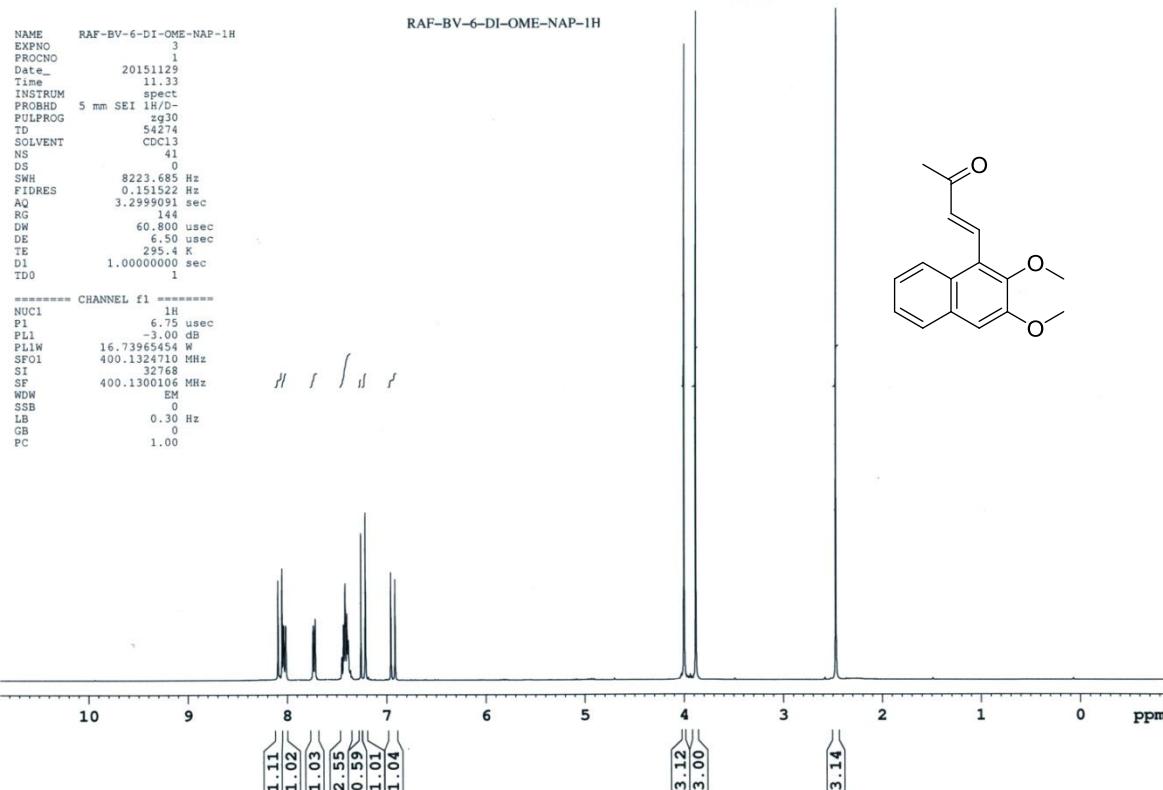
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 2h**



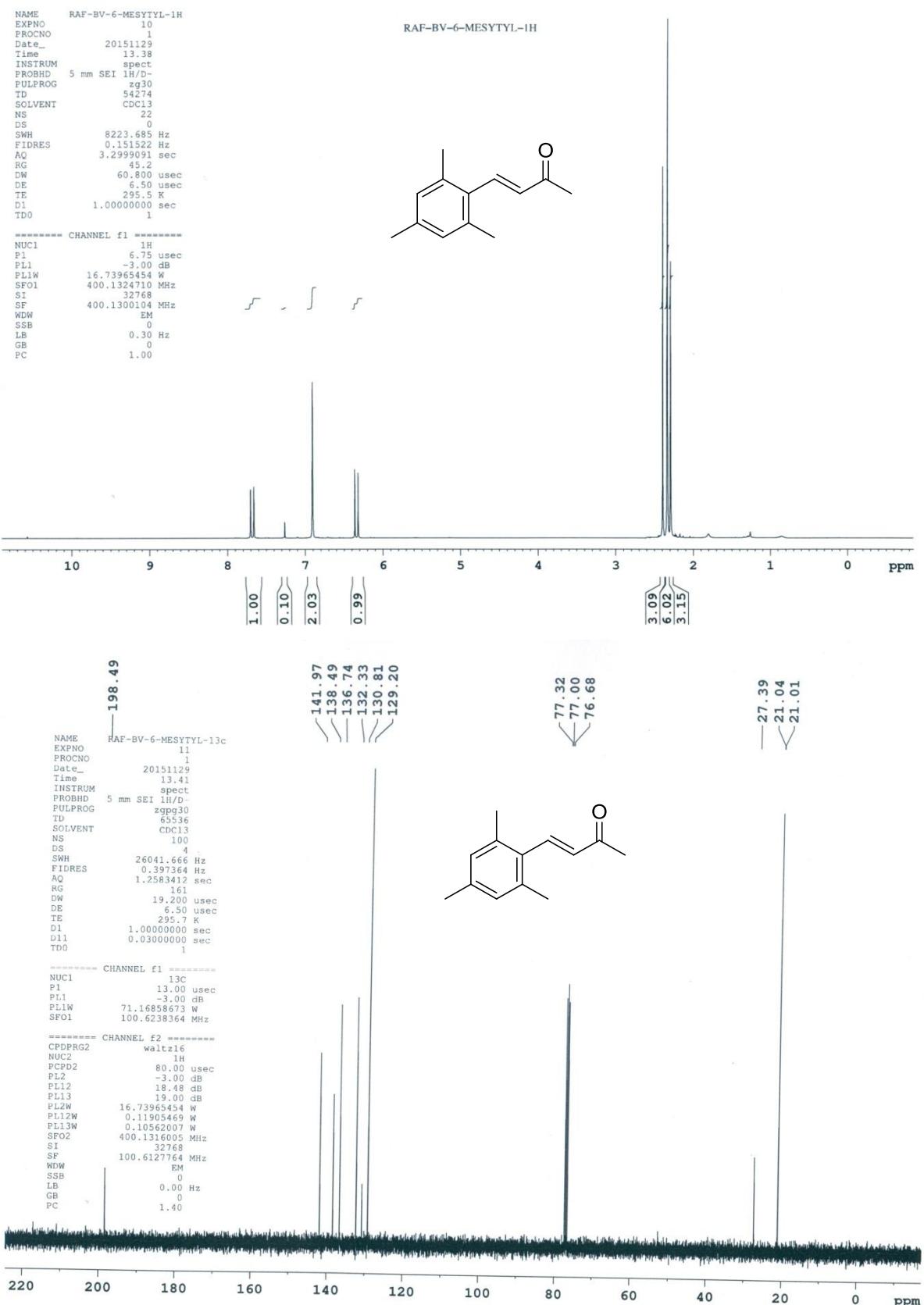
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 2i**



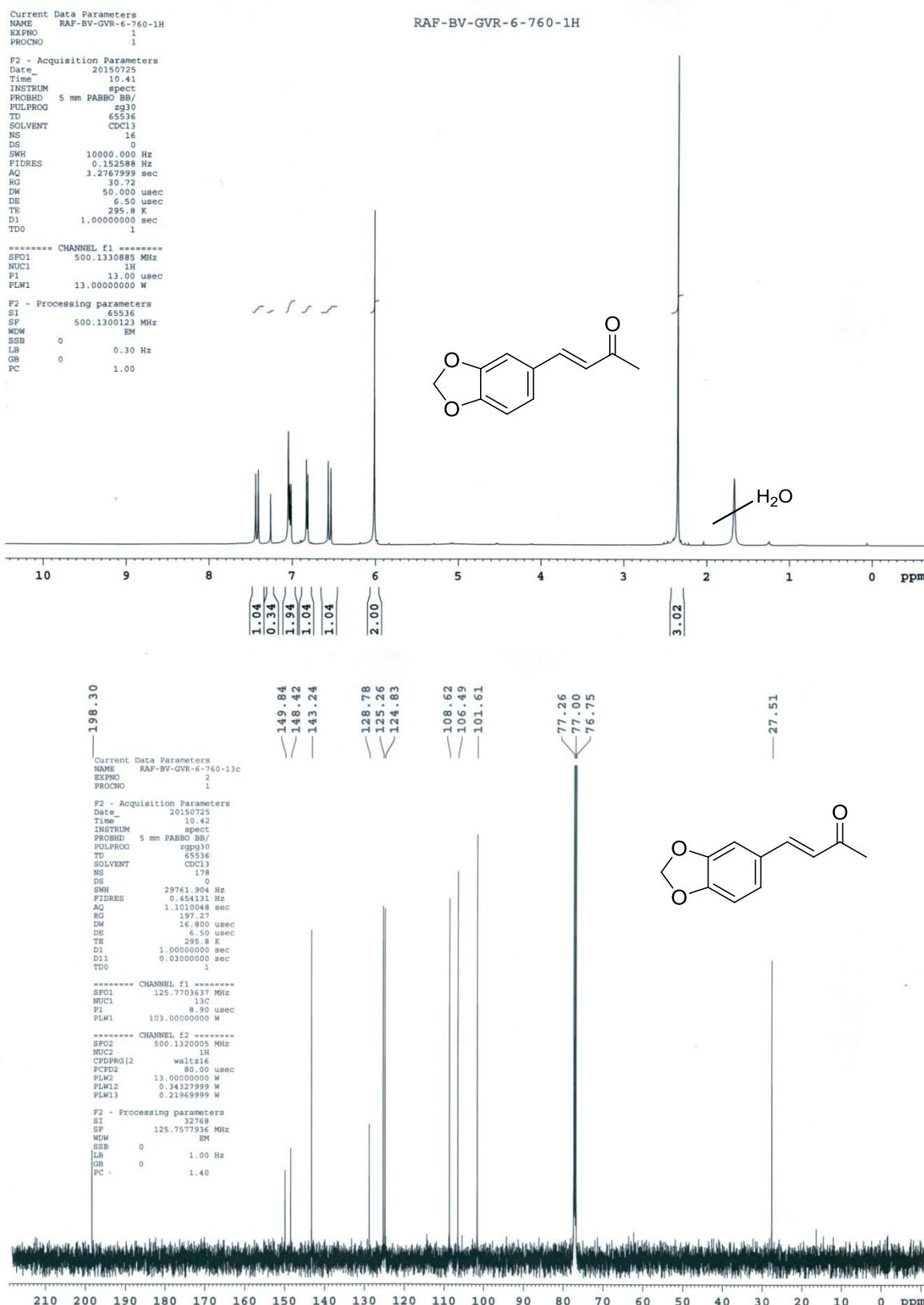
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 2j**



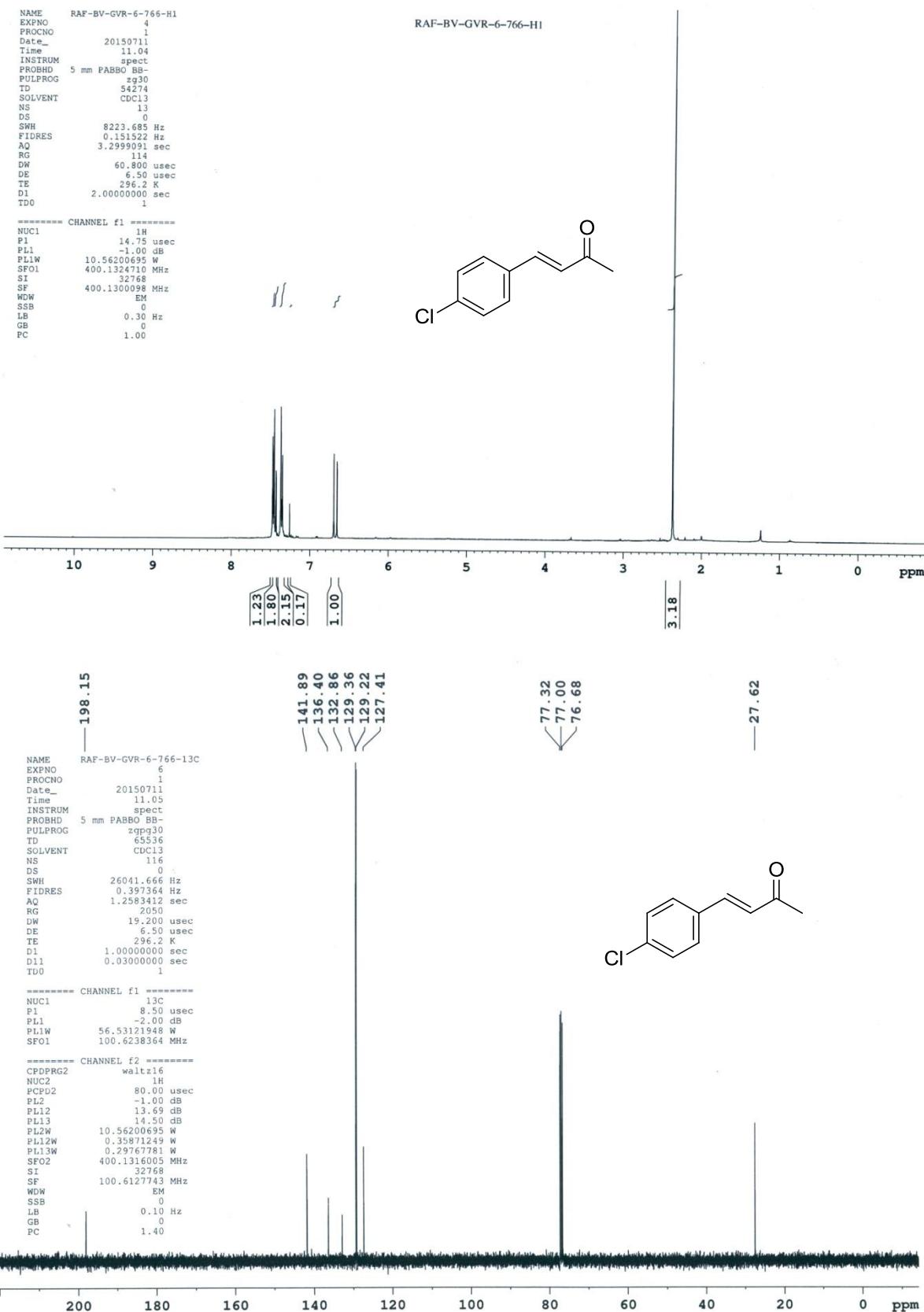
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 2k**



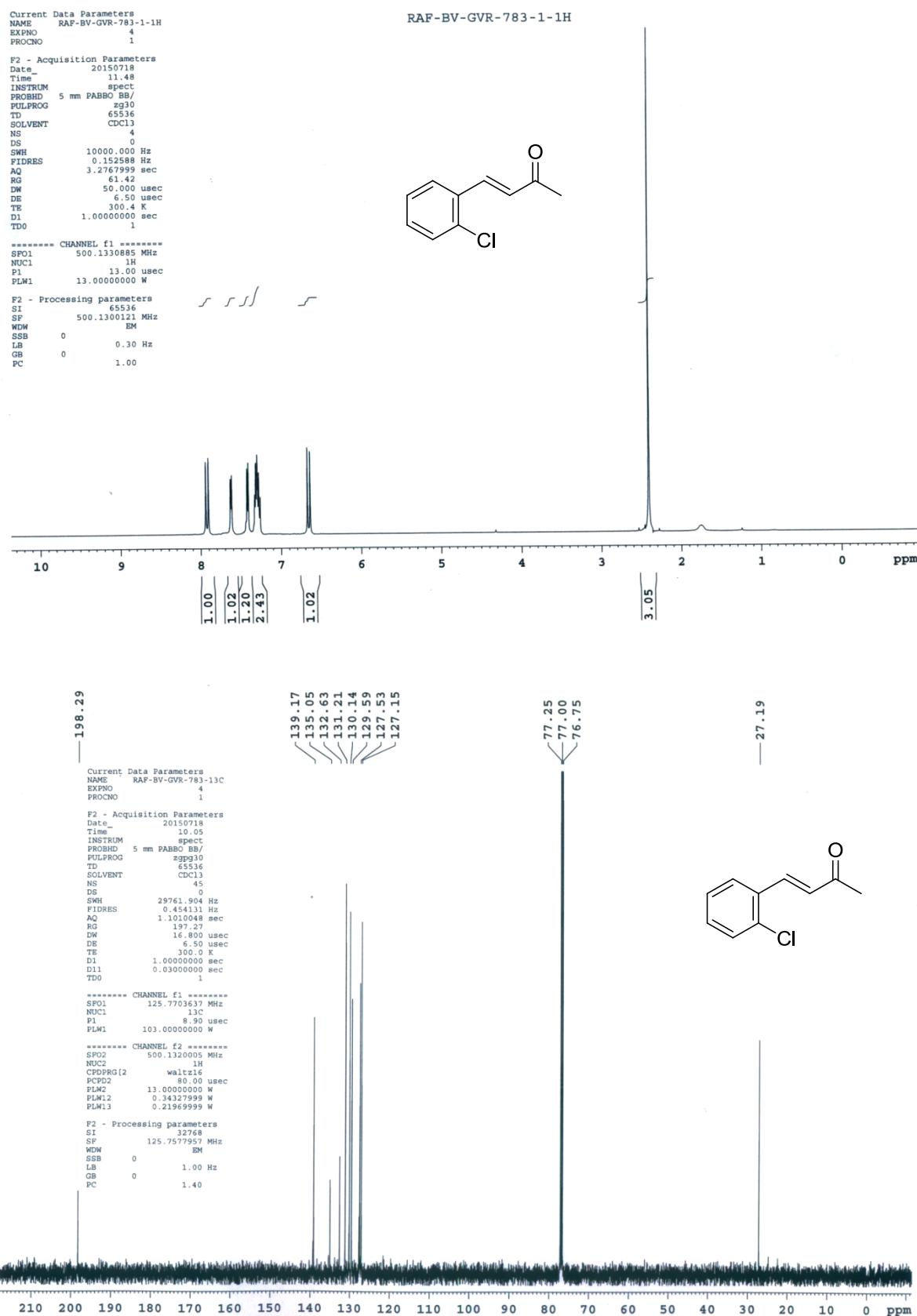
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 2l**



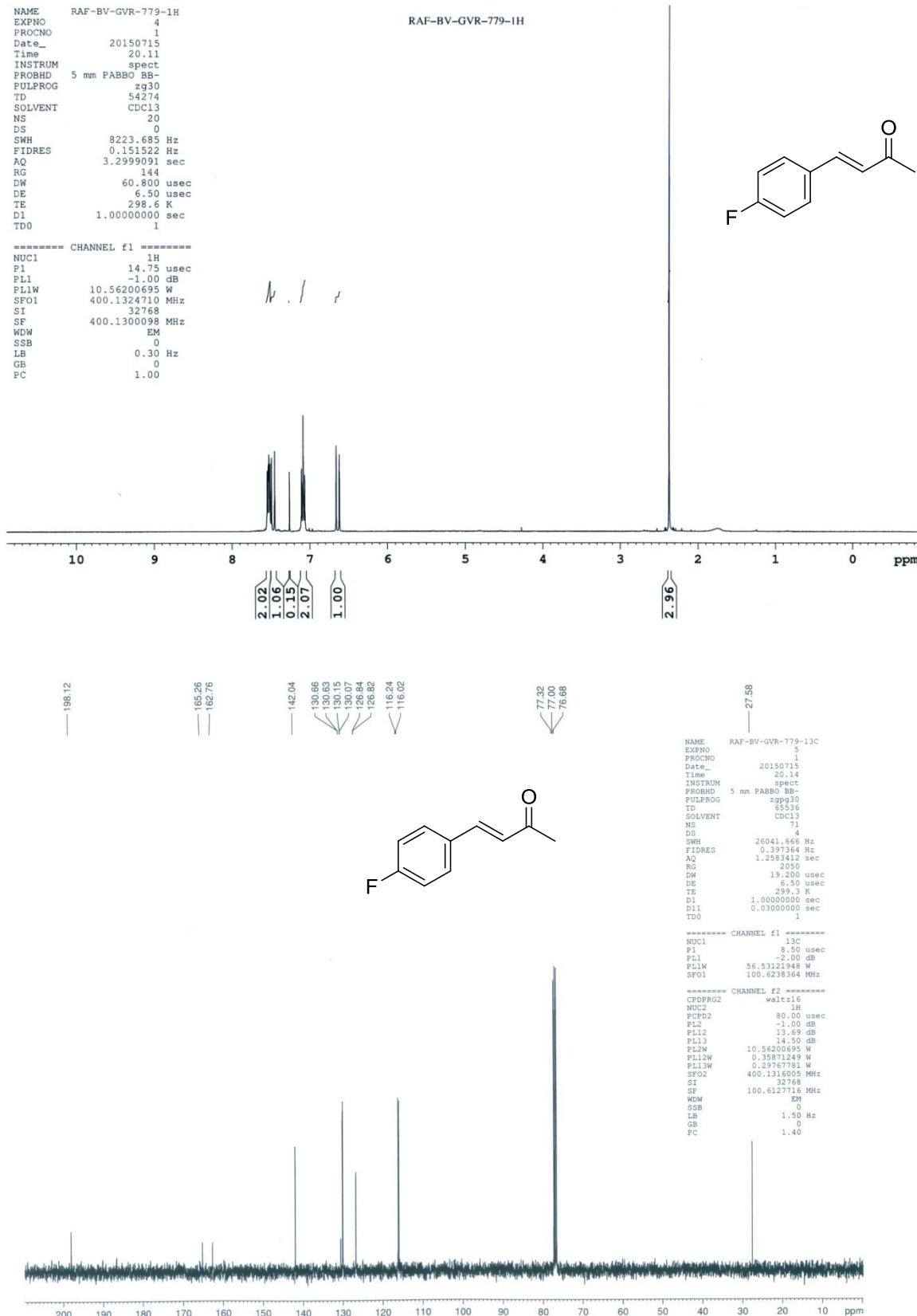
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 2m**



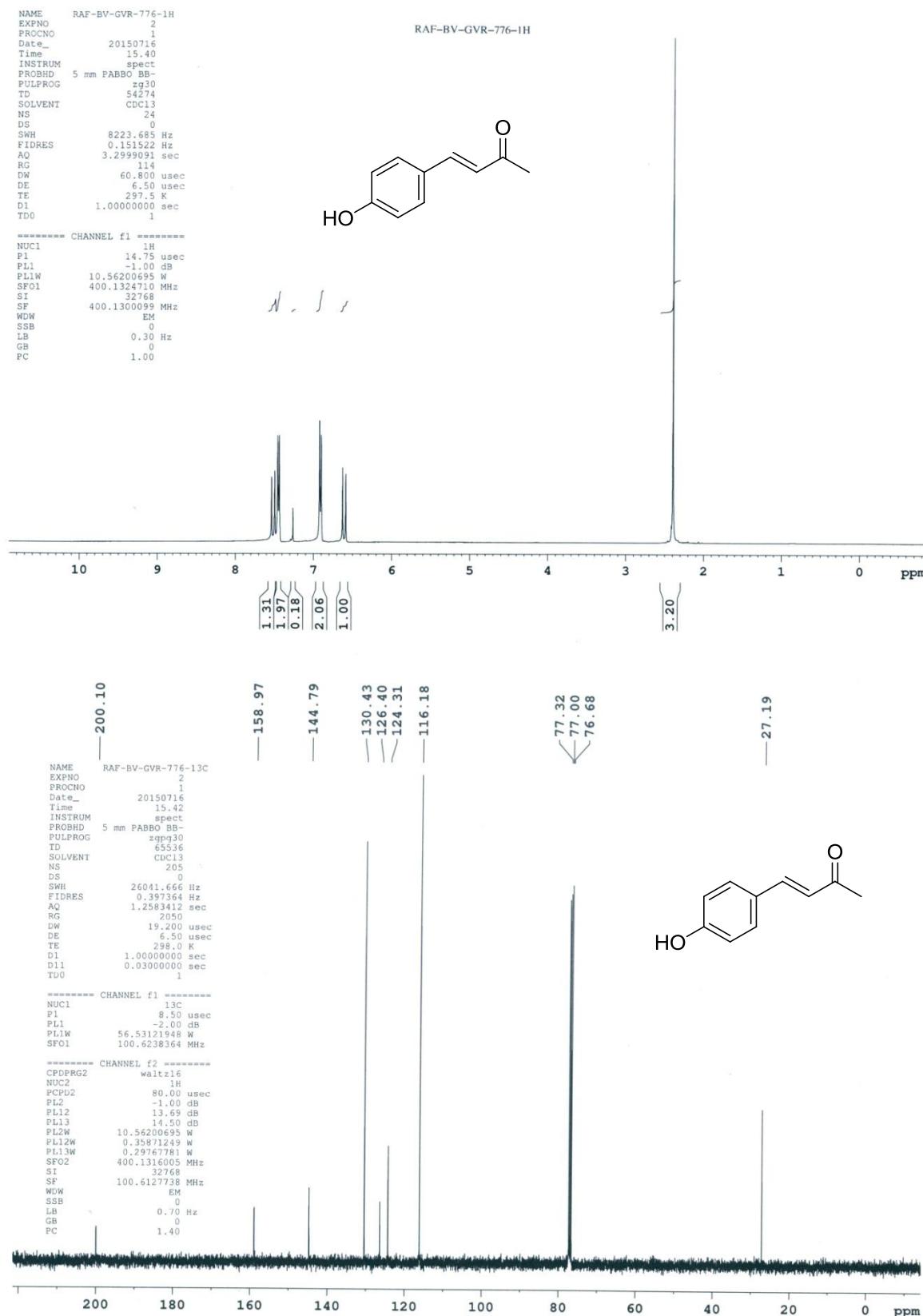
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 2n**



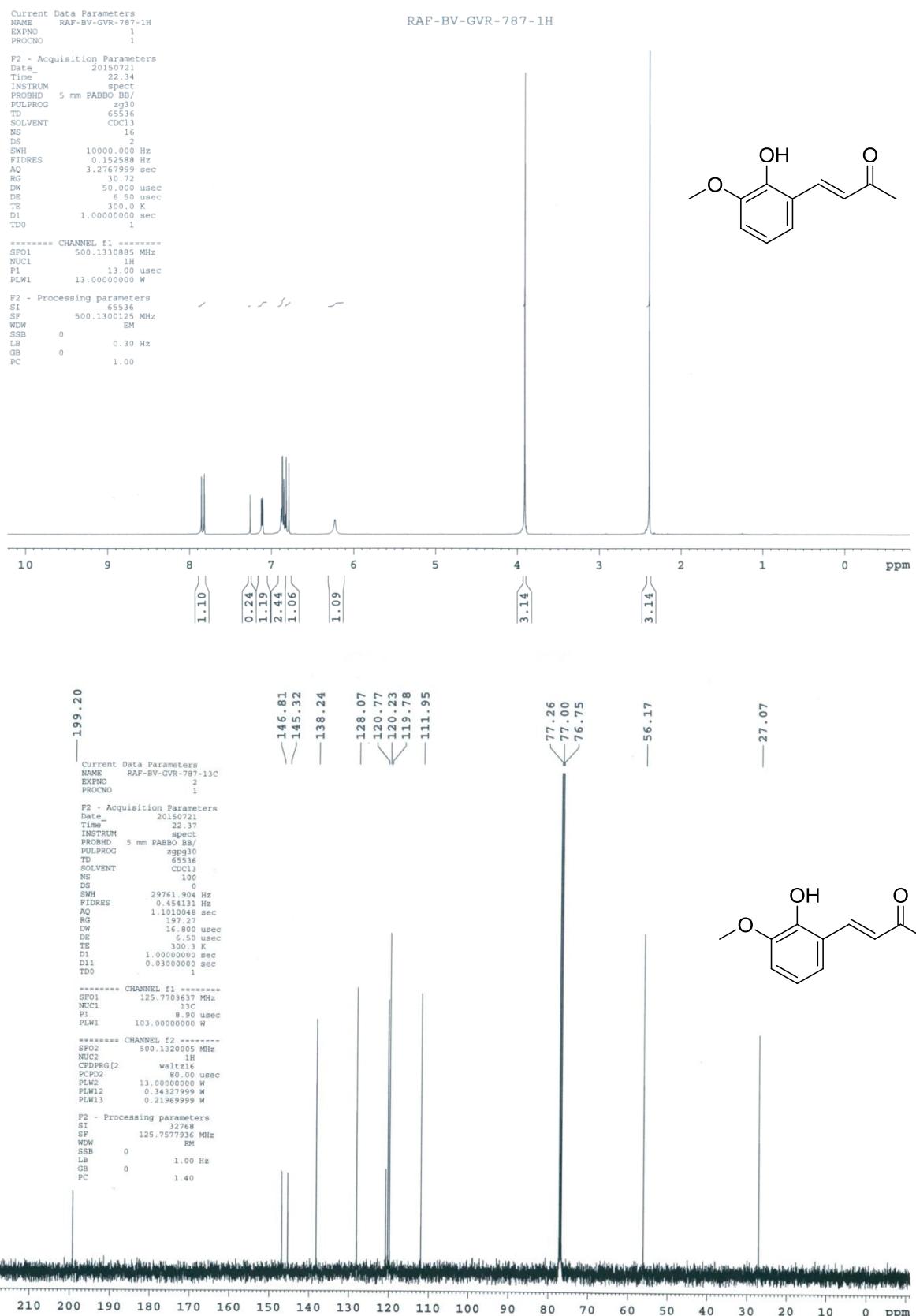
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 2o**



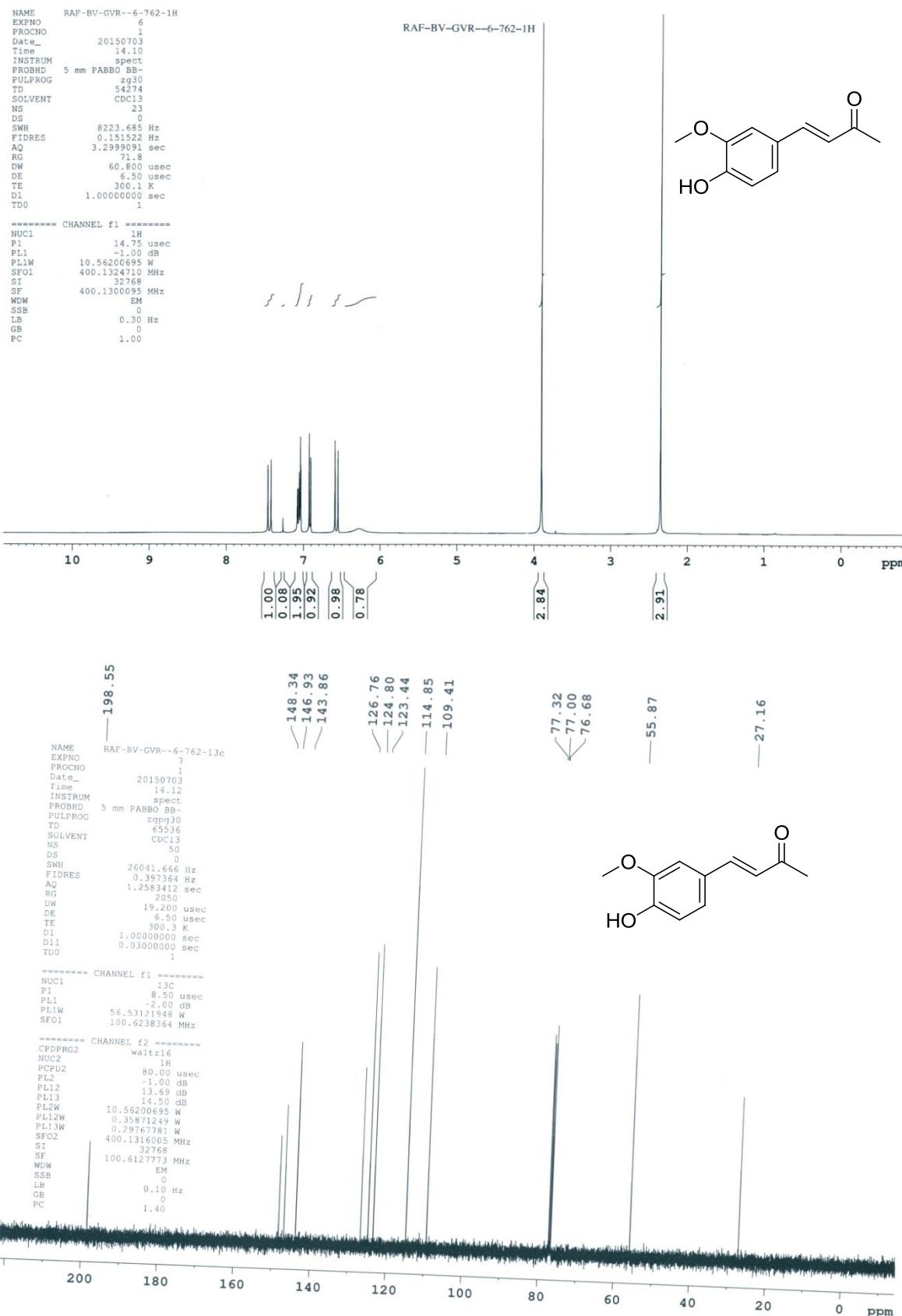
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 2p**



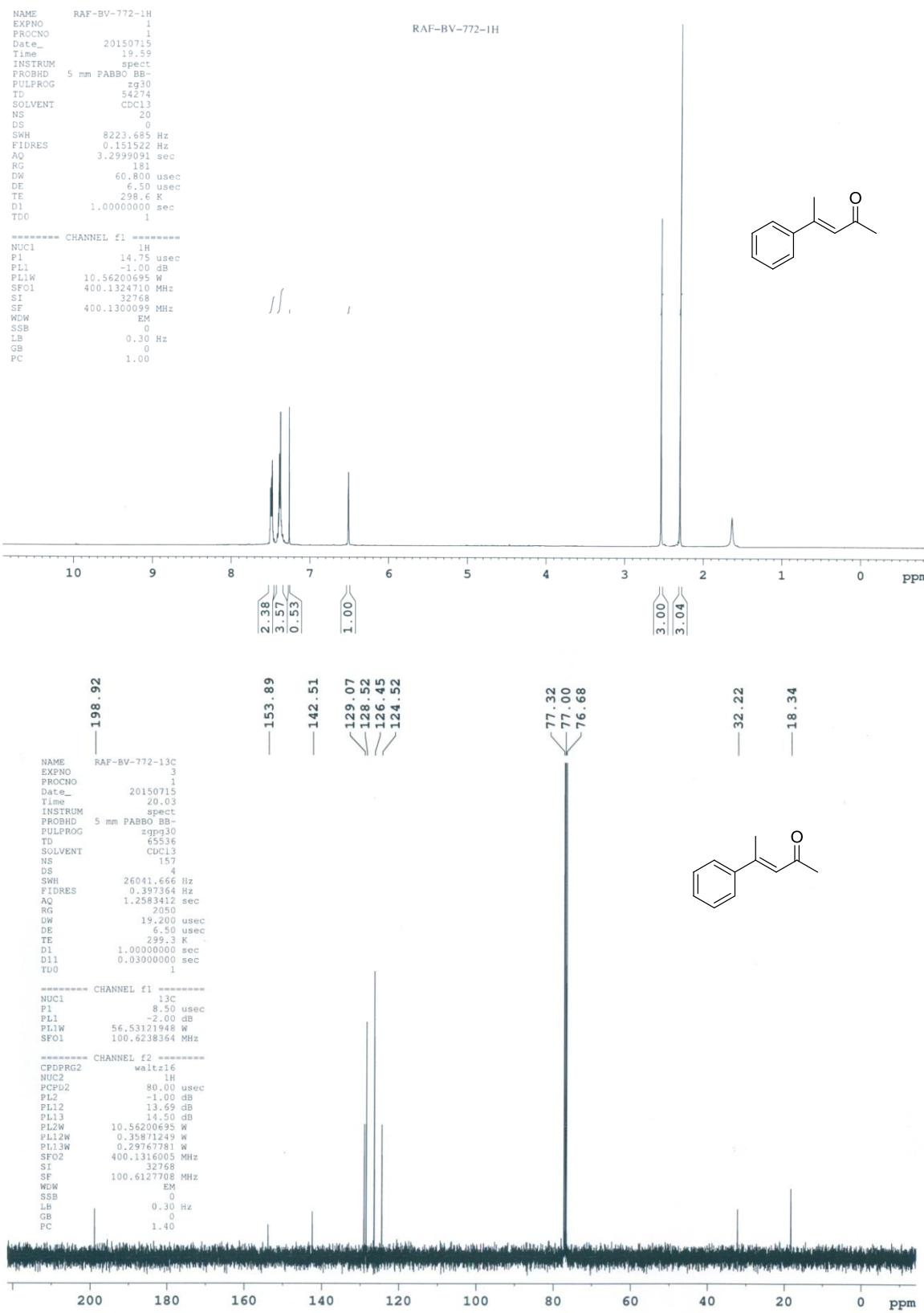
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 2q**



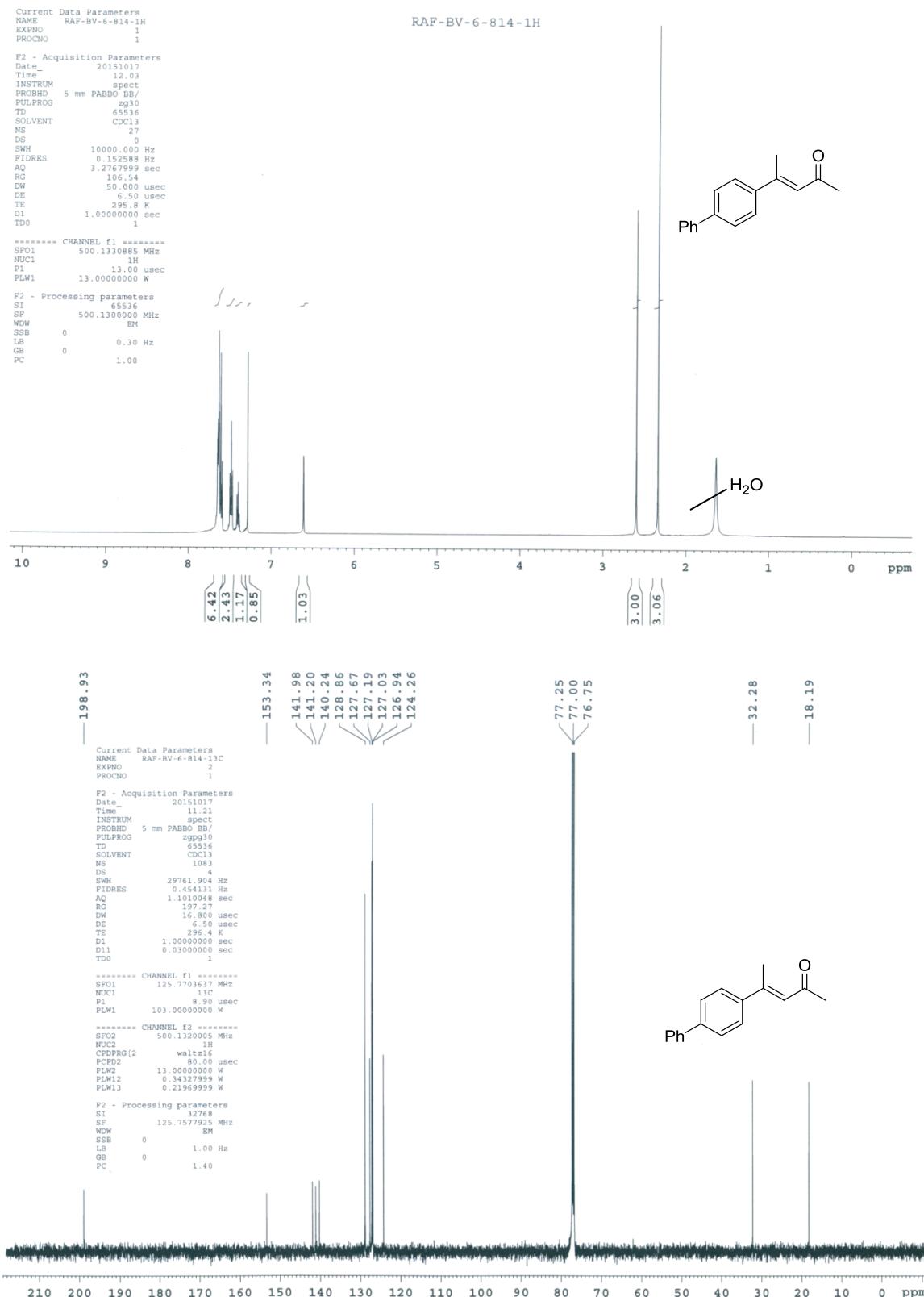
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 2r**



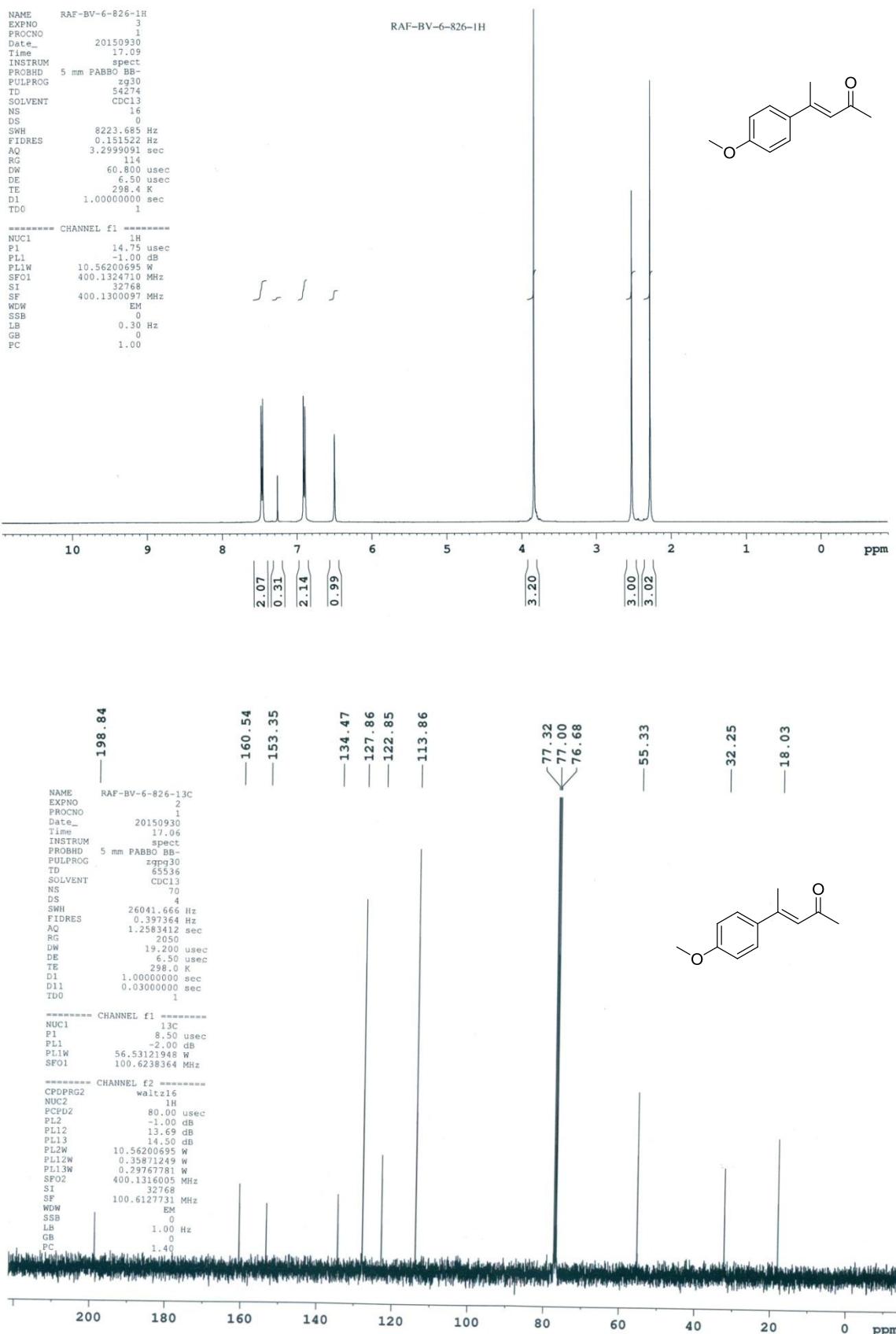
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 4a**



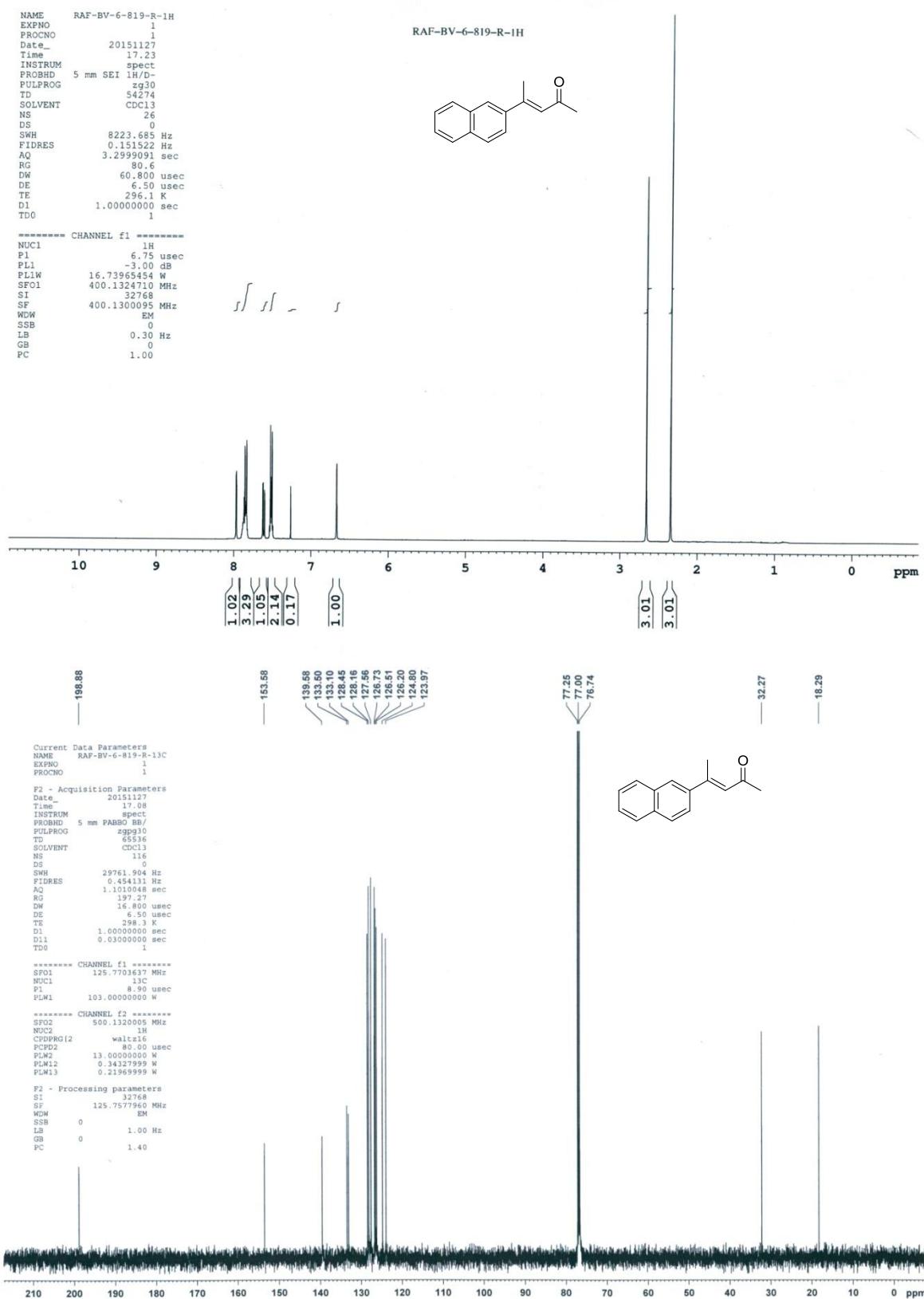
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 4b**



**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 4c**



**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 4d**



**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 4e**

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NAME      RAF-BV-6-822-UP-1H
EXPNO        1
PROCNO       1
Date_ 20151029
Time   19.16
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PROBHD  5 mm SEI 1H/D-
PULPROG  zg30
TD      54274
SOLVENT   CDCl3
NS       33
DS        0
SWH     8223.685 Hz
FIDRES    0.151522 Hz
AQ      3.299994 sec
RG      60.800 usec
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TE      295.3 K
D1      1.0000000 sec
TDO      1

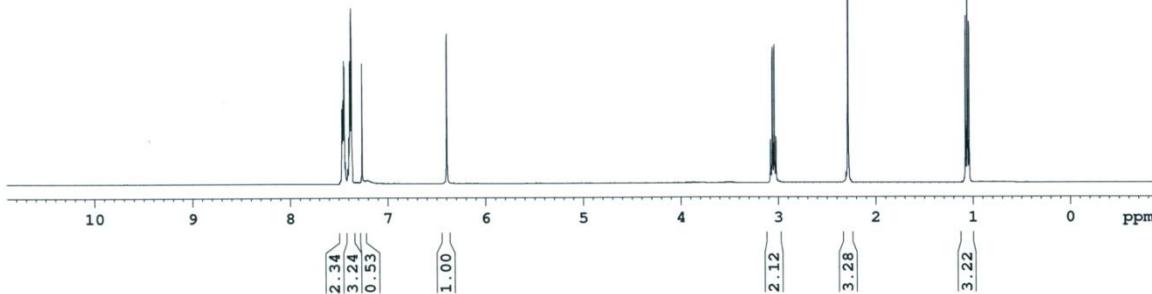
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RAF-BV-6-822-UP-1H

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SF     400.1300102 MHz
WDW        EM
SSB        0
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PC      1.00

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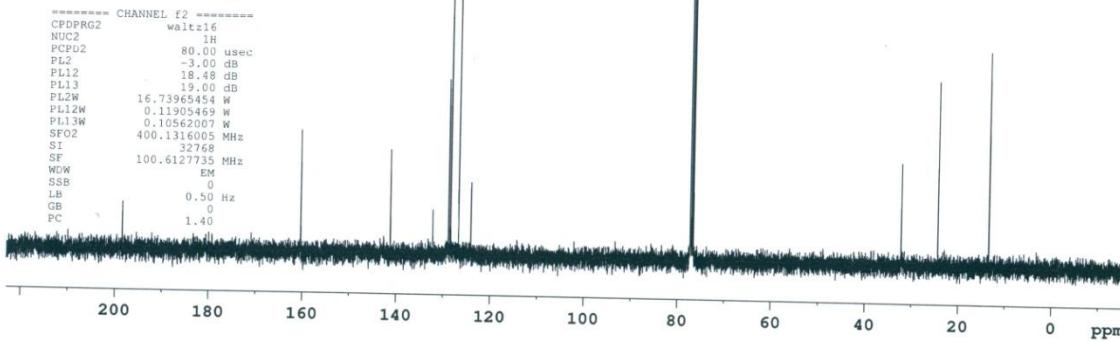
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PROCNO       1
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Time   19.20
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PULPROG  zgpg30
TD      65536
SOLVENT   CDCl3
NS       417
DS        4
SWH     26041.666 Hz
FIDRES    0.397364 Hz
AQ      1.2583412 sec
RG      32
DW      19.200 usec
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TE      295.3 K
D1      1.0000000 sec
D1L     0.03000000 sec
TDO      1

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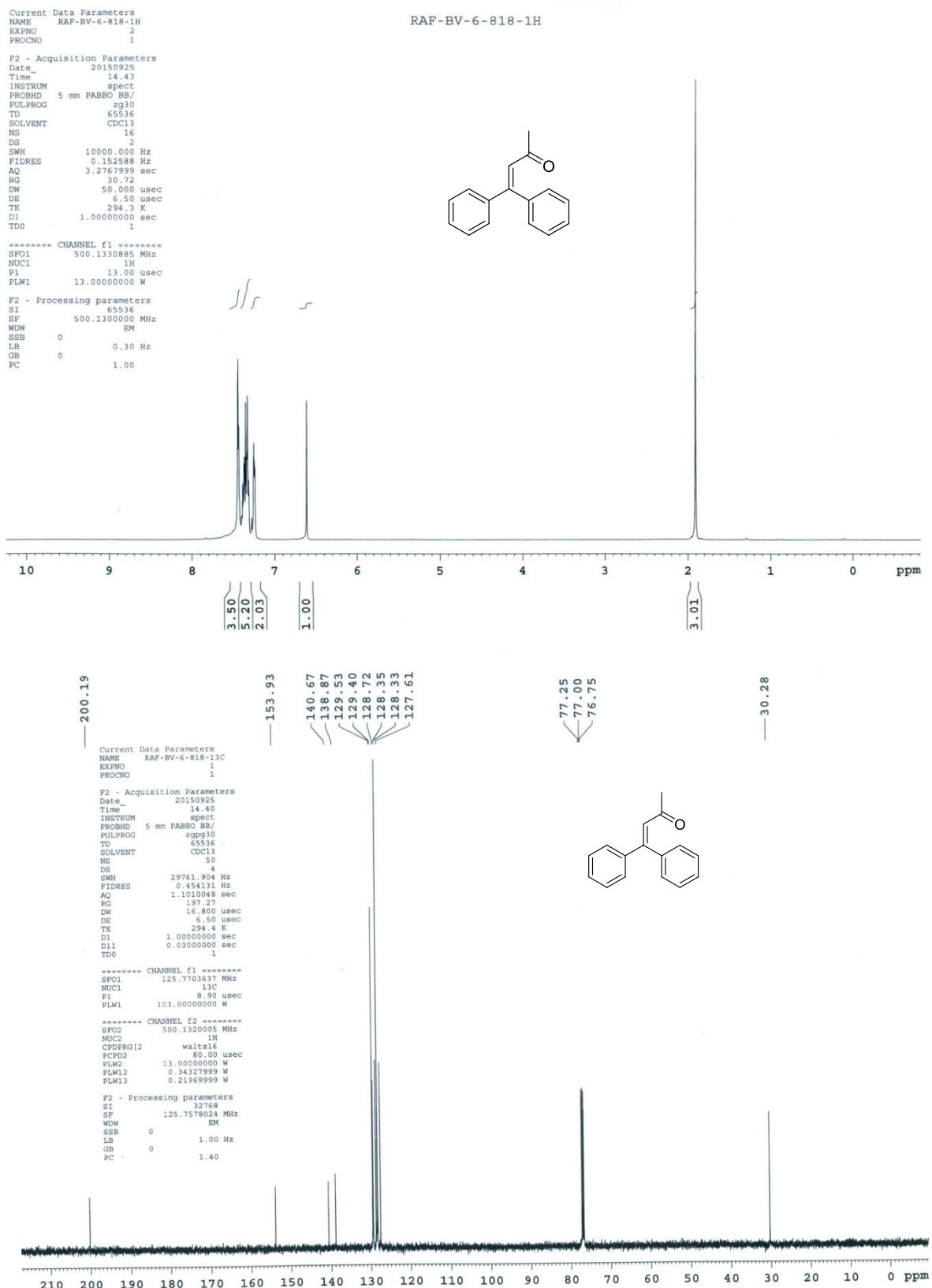
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PL1      -3.00 dB
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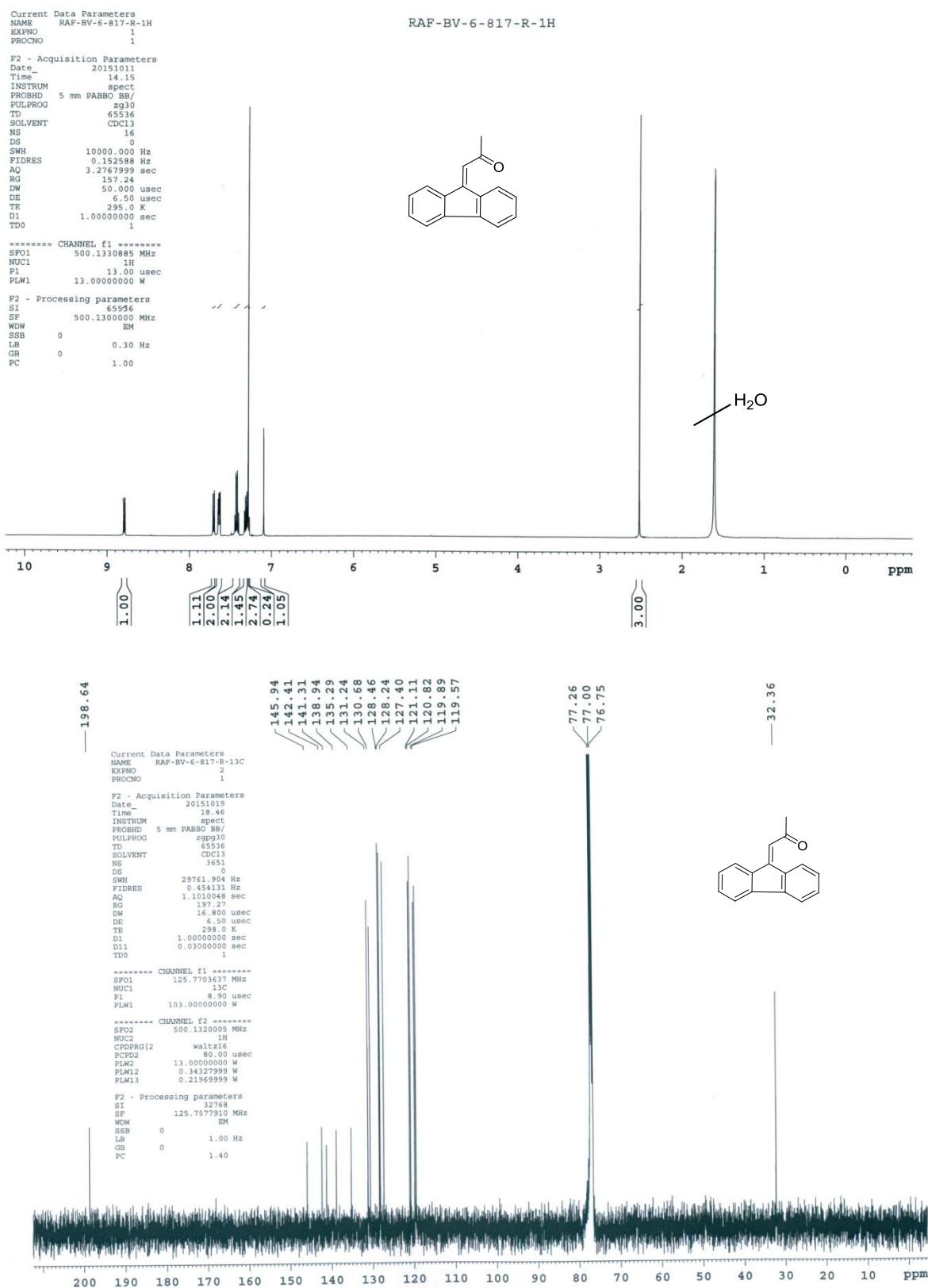
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**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 4f**



**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 4g**



**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 6a**

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PROCNO 1

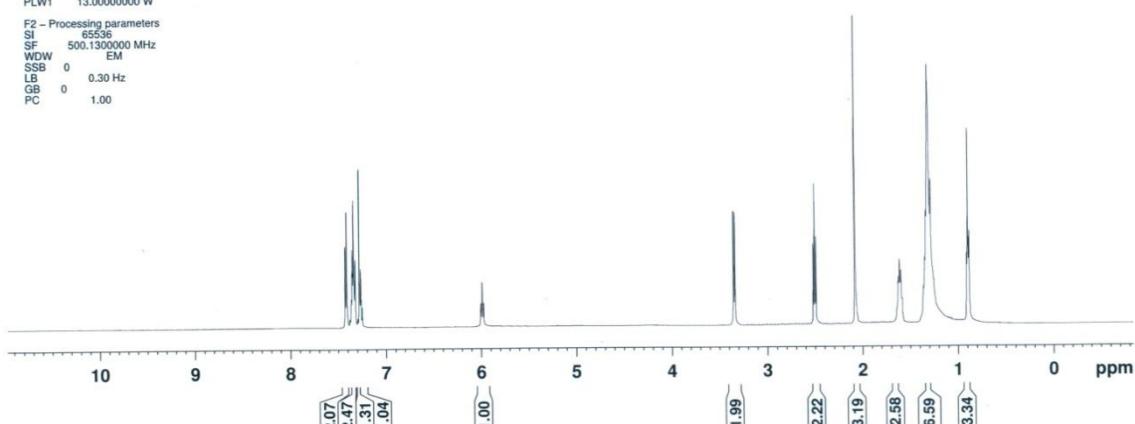
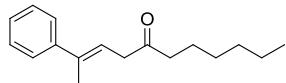
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TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 16  
DS 2  
SWH 10000.000 Hz  
FIDRES 0.152588 Hz  
AQ 3.276589 sec  
RG 30.72  
DW 50.000 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL F1 =====

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P1 13.00 usec  
PLW1 13.0000000 W

F2 - Processing parameters  
SI 65536  
SF 500.1300000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



— 208.95

Current Data Parameters  
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EXPNO 6  
PROCNO 1

F2 - Acquisition Parameters  
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Time 23:53  
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PULPROG zgpp30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 110  
DS 2  
SWH 29781.904 Hz  
FIDRES 0.454131 Hz  
AQ 1.101048 sec  
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D11 0.032768000 sec  
TDO 1

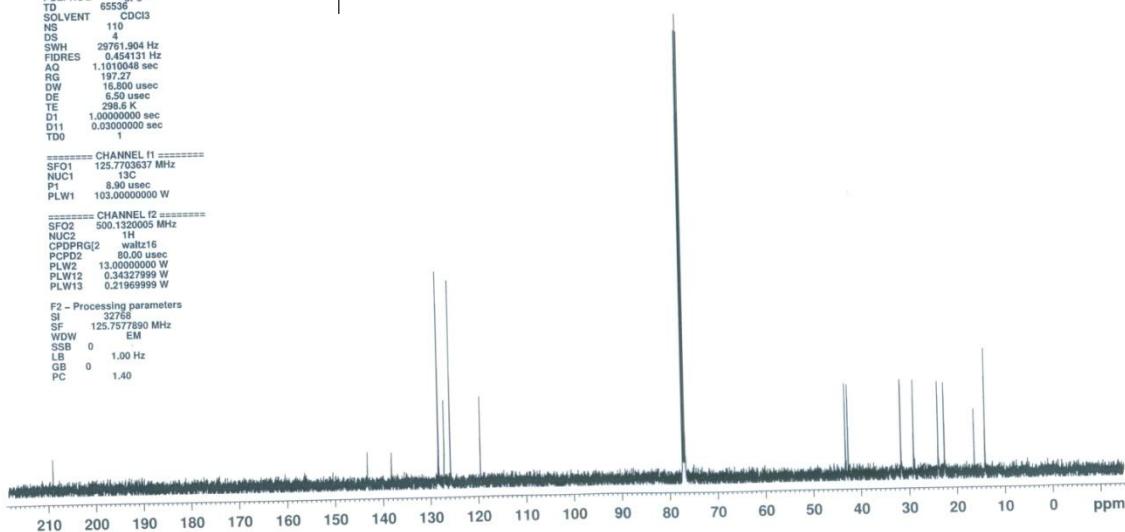
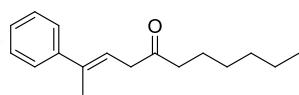
===== CHANNEL F1 =====

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NUC1 <sup>13</sup>C  
P1 8.90 usec  
PLW1 103.0000000 W

===== CHANNEL F2 =====

SFO2 500.1320000 MHz  
NUC2 <sup>1</sup>H  
CPDPRG[2] waltz16  
PCP[2] 80.00 usec  
PLW2 13.0000000 W  
PLW12 0.34327999 W  
PLW13 0.21969999 W

F2 - Processing parameters  
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SF 125.7574900 MHz  
WOW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 6b**

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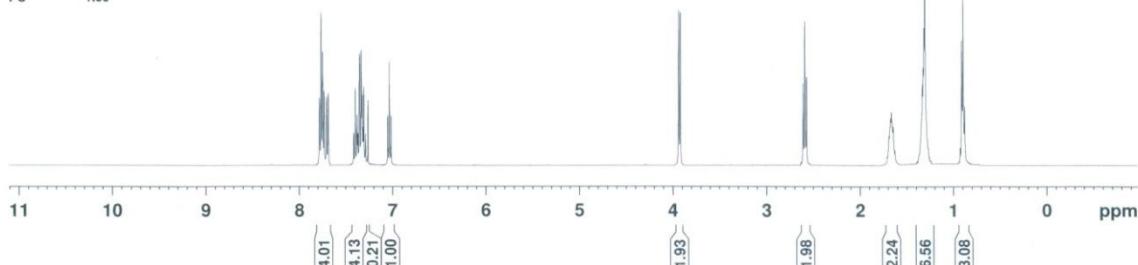
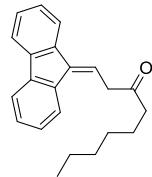
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 Time 7.07  
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 PULPROG zg30  
 TD 54274  
 SOLVENT CDCl<sub>3</sub>  
 NS 31  
 DS 0  
 SWH 8223.685 Hz  
 FIDRES 0.151522 Hz  
 AQ 3.2998593 sec  
 RG 57  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 294.6 K  
 D1 1.0000000 sec  
 TDO 1  
 FID0 1

===== CHANNEL f1 ======

NUC1 <sup>1</sup>H  
 P1 6.75 usec  
 PL1 -3.00 dB  
 PL1W 16.73965454 W  
 SF01 400.1324710 MHz

F2 - Processing parameters  
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 SF 400.1300095 MHz  
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207.29

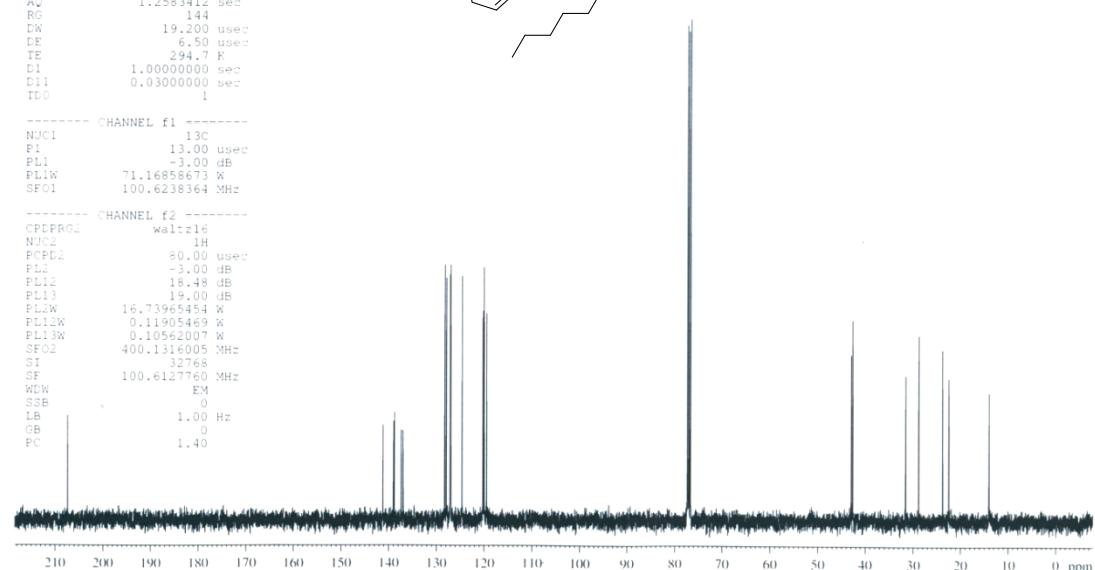
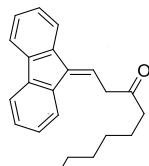
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 Time 13.40  
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 PULPROG zg30  
 Tt 65536  
 SOLVENT CDCl<sub>3</sub>  
 NS 200  
 DS 4  
 SWH 26041.664 Hz  
 FIDRES 0.397364 Hz  
 AQ 1.2583412 sec  
 RG 144  
 DW 19.200 usec  
 DE 6.50 usec  
 TE 294.7 K  
 D1 1.0000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 ======

NUC1 <sup>13</sup>C  
 P1 13.00 usec  
 PL1 -3.00 dB  
 PL1W 71.16858673 W  
 SF01 100.6238364 MHz

===== CHANNEL f2 ======

CPDPRG waltz16  
 NUC2 <sup>1</sup>H  
 PCPD2 80.00 usec  
 PL2 -3.00 dB  
 PL2 13.48 dB  
 PL13 19.00 dB  
 PL1W 16.73965454 W  
 PL1W 0.11905469 W  
 PL13W 0.10562007 W  
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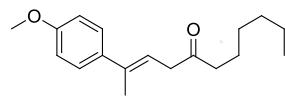
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 6c**

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RAF-BV-6-855-DN-1H

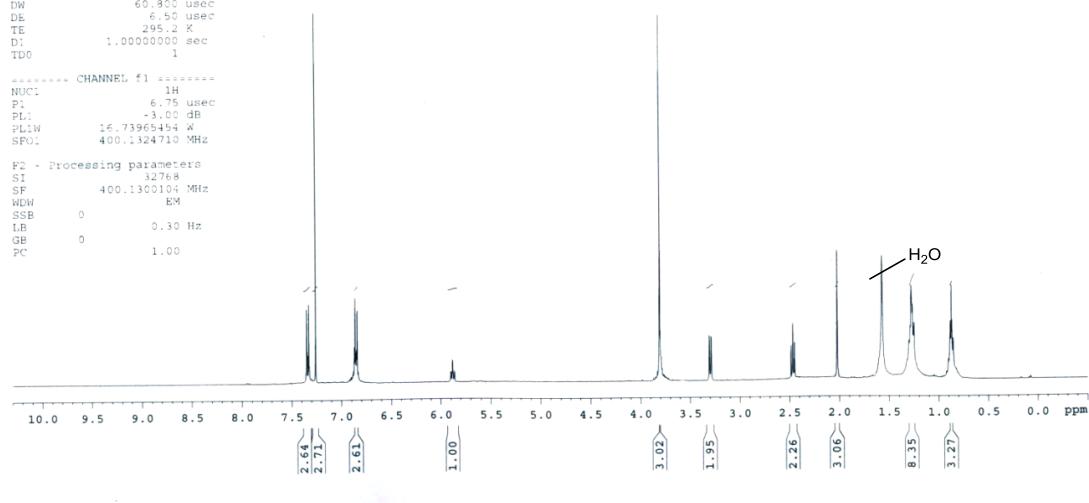
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 PULPROG zg30  
 TD 54274  
 SOLVENT CDCl<sub>3</sub>  
 NS 120  
 DS 0  
 SWH 8221.685 Hz  
 FIDRES 0.151522 Hz  
 AQ 3.2998593 sec  
 RG 204  
 DW 60.800 usec  
 DE 6.50 usec  
 TE 295.2 K  
 D1 1.0000000 sec  
 TDO 1



\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
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 P1 6.75 usec  
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 PL1W 16.73965454 W  
 SFO1 400.1324710 MHz

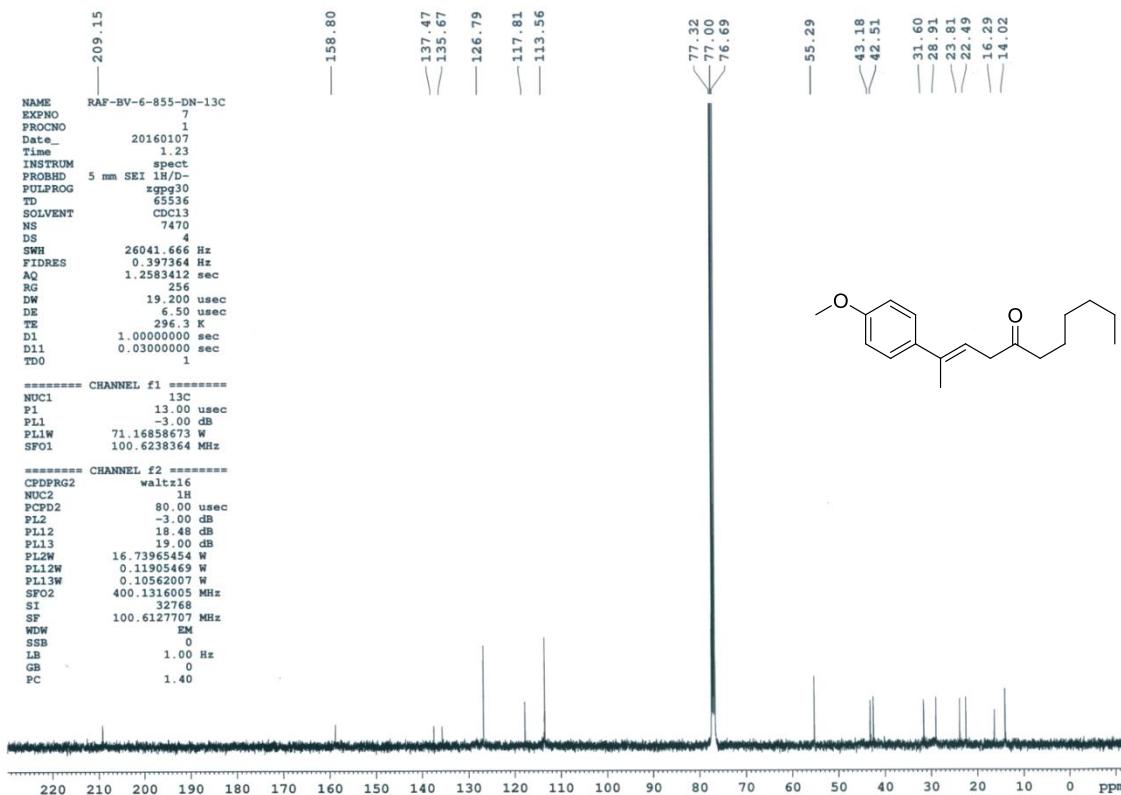
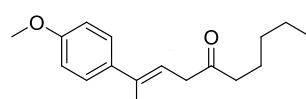
F2 - Processing parameters  
 SI 32768  
 SF 400.1300104 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



NAME RAF-BV-6-855-DN-13C  
 EXPNO 7  
 PROCNO 1  
 Date 20160107  
 Time 1.23  
 INSTRUM spect  
 PROBHD 5 mm SEI 1H/D-  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl<sub>3</sub>  
 NS 7470  
 DS 4  
 SWH 26041.666 Hz  
 FIDRES 0.397500 Hz  
 AQ 1.2583412 sec  
 RG 256  
 DW 19.200 usec  
 DE 6.50 usec  
 TE 296.3 K  
 D1 1.0000000 sec  
 D11 0.03000000 sec  
 TDO 1

\*\*\*\*\* CHANNEL f1 \*\*\*\*\*  
 NUC1 13C  
 P1 13.00 usec  
 PL1 -3.00 dB  
 PL1W 71.16858673 W  
 SFO1 100.6238364 MHz

\*\*\*\*\* CHANNEL f2 \*\*\*\*\*  
 CPDPRG2 waltz16  
 NUC2 1H  
 PCPD2 80.00 usec  
 PL2 -3.00 dB  
 PL12 18.48 dB  
 PL13 1.00 dB  
 PL12W 16.73965454 W  
 PL13W 0.11905469 W  
 PL13W 0.10562007 W  
 SFO2 400.1316005 MHz  
 SI 32768  
 SF 100.6127707 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 6d**

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Current Data Parameters
NAME RAF-BV-6-869-1H
EXPNO 1
PROCNO 1

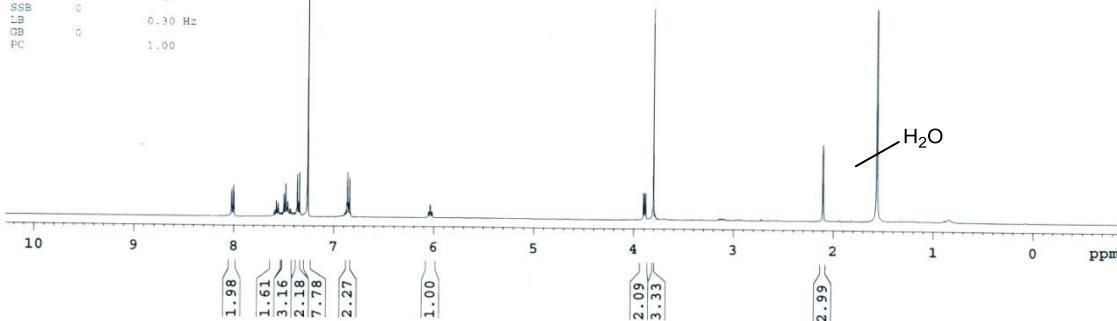
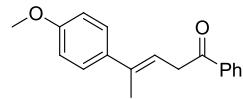
F2 - Acquisition Parameters
Date 20160125
Time 8.22
INSTRUM spect
PROBHD 5 mm SEI 1H/D-
PULPROG zg30
TD 54274
SOLVENT CDCl3
NS 6
DS 0
SWH 8223.685 Hz
FIDRES 0.151522 Hz
AQ 3.2998593 sec
RG 512
DW 60.800 usec
DE 6.50 usec
TE 295.1 K
D1 1.0000000 sec
TDD 1

***** CHANNEL F1 *****
NUC1 1H
P1 6.75 usec
PL1 -3.00 dB
PL1W 16.73965454 W
SF01 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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RAF-BV-6-869-1H



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Current Data Parameters
NAME RAF-BV-6-869-13C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date 20160125
Time 8.41
INSTRUM spect
PROBHD 5 mm PABBO BB
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 200
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.0100448 sec
RG 128
DW 16.800 usec
DE 6.50 usec
TE 297.1 K
D1 1.0000000 sec
D1L 0.01000000 sec
TDD 1

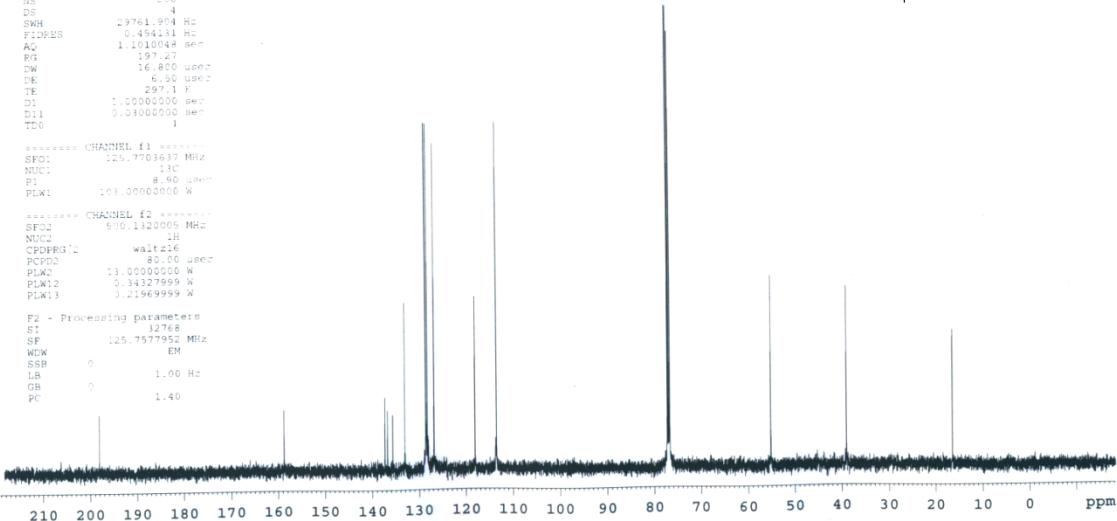
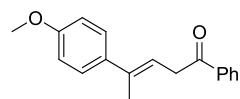
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SF01 125.7703617 MHz
NUC1 13C
P1 8.90 usec
PL1 103.0000000 W

***** CHANNEL F2 *****
SF02 600.1320000 MHz
NUC2 1H
CPDPG2 1 wait216
CPDPG2 80.00 usec
PLX2 13.0000000 W
PLX12 0.34327999 W
PLX13 0.25969999 W

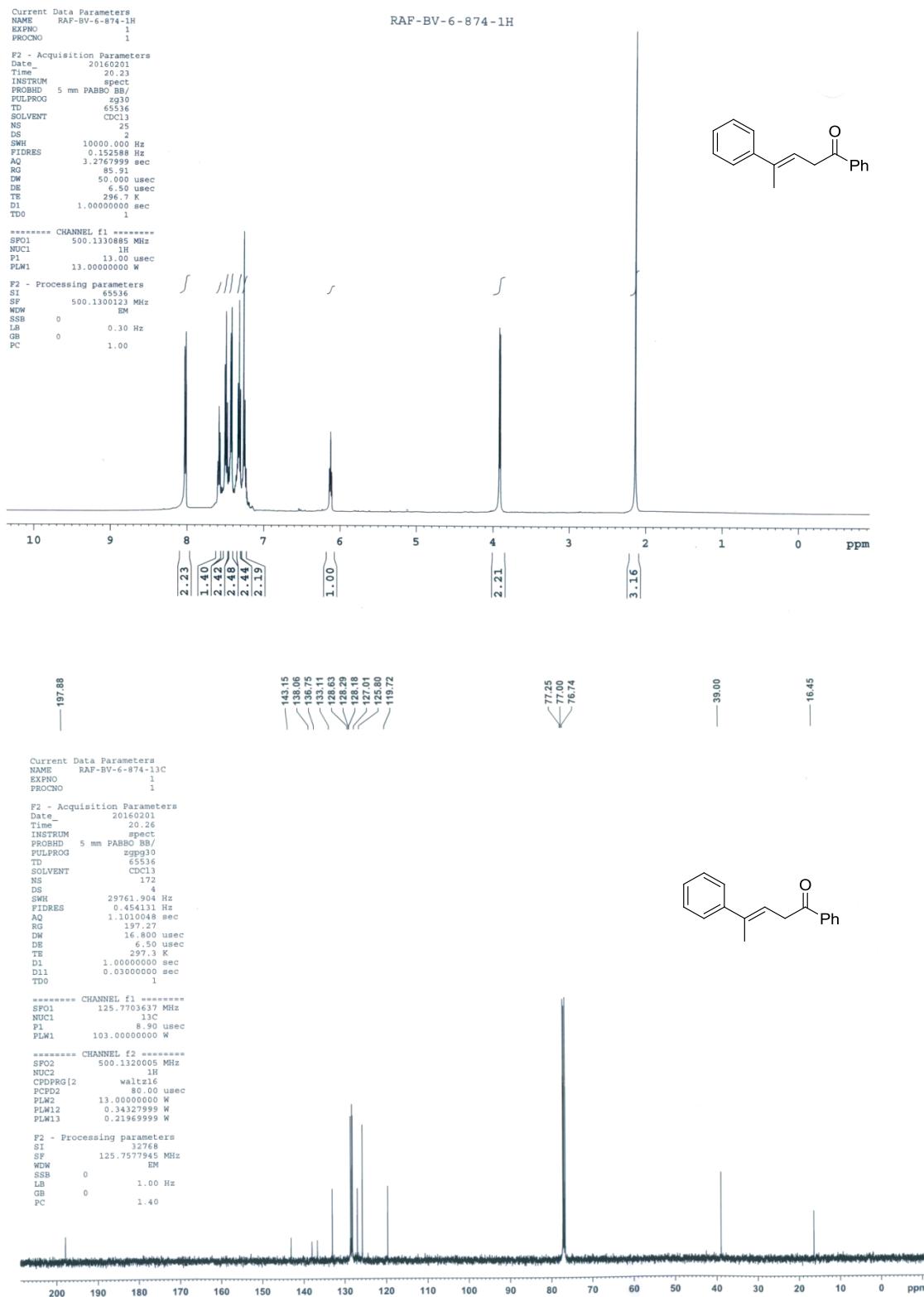
F2 - Processing parameters
SI 32768
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WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

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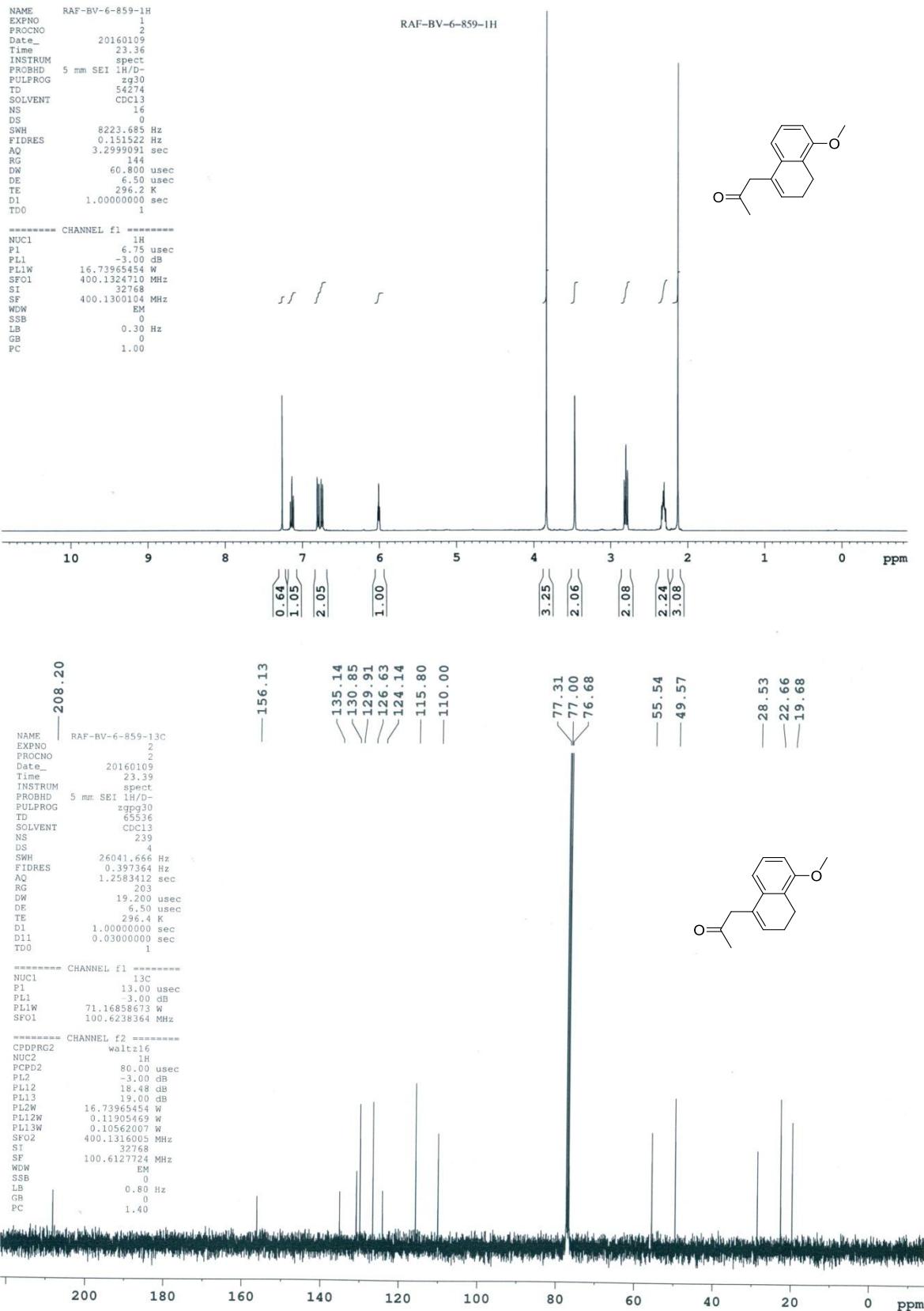
198.03 ——————  
158.77 ——————  
137.36 /—————  
136.77 /—————  
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133.06 /—————  
128.61 /—————  
128.28 /—————  
126.82 /—————  
118.08 /—————  
113.52 /—————  
77.25 /—————  
77.00 /—————  
76.75 /—————  
55.25 ——————  
39.02 ——————  
16.44 ——————



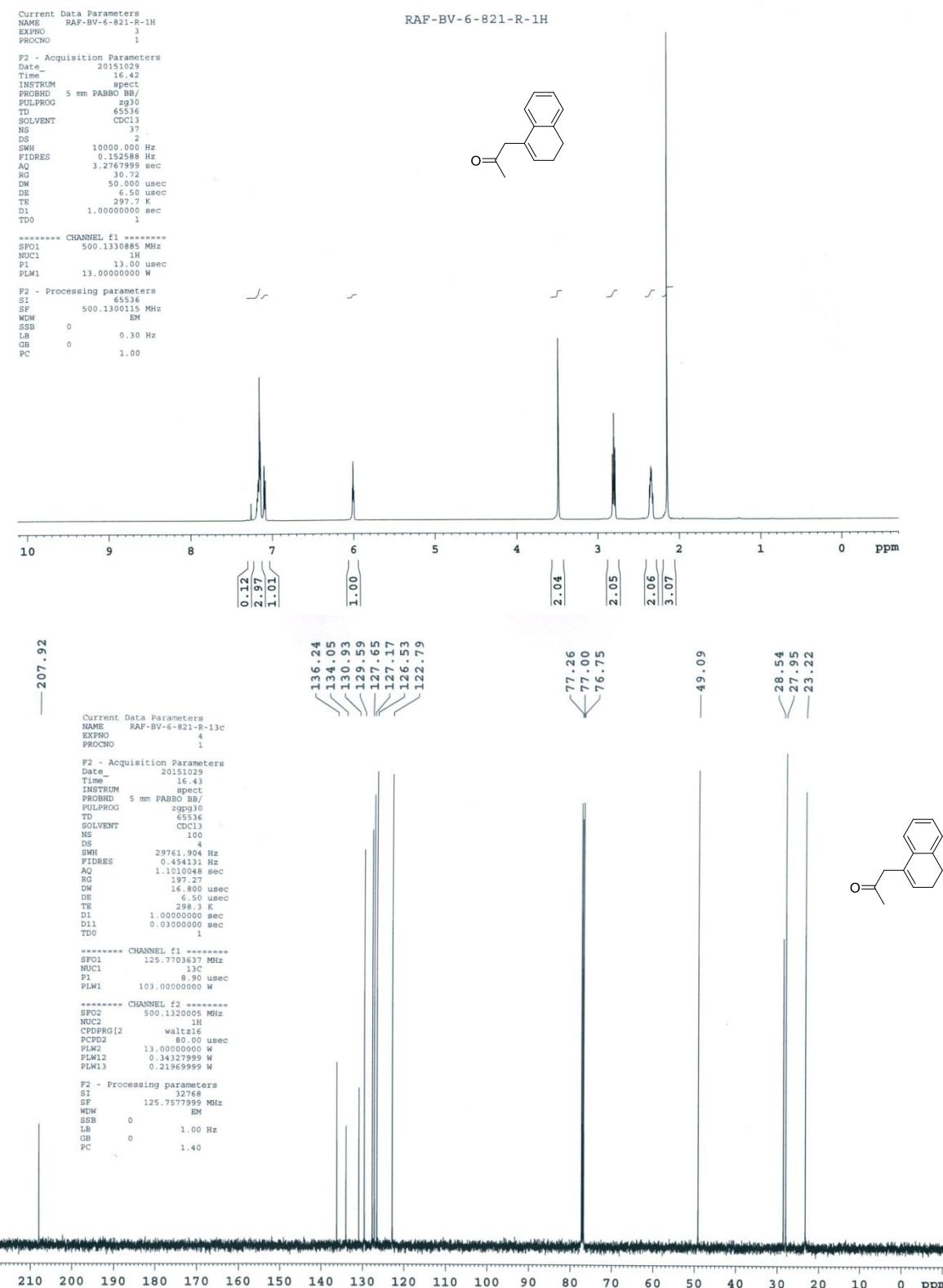
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 6e**



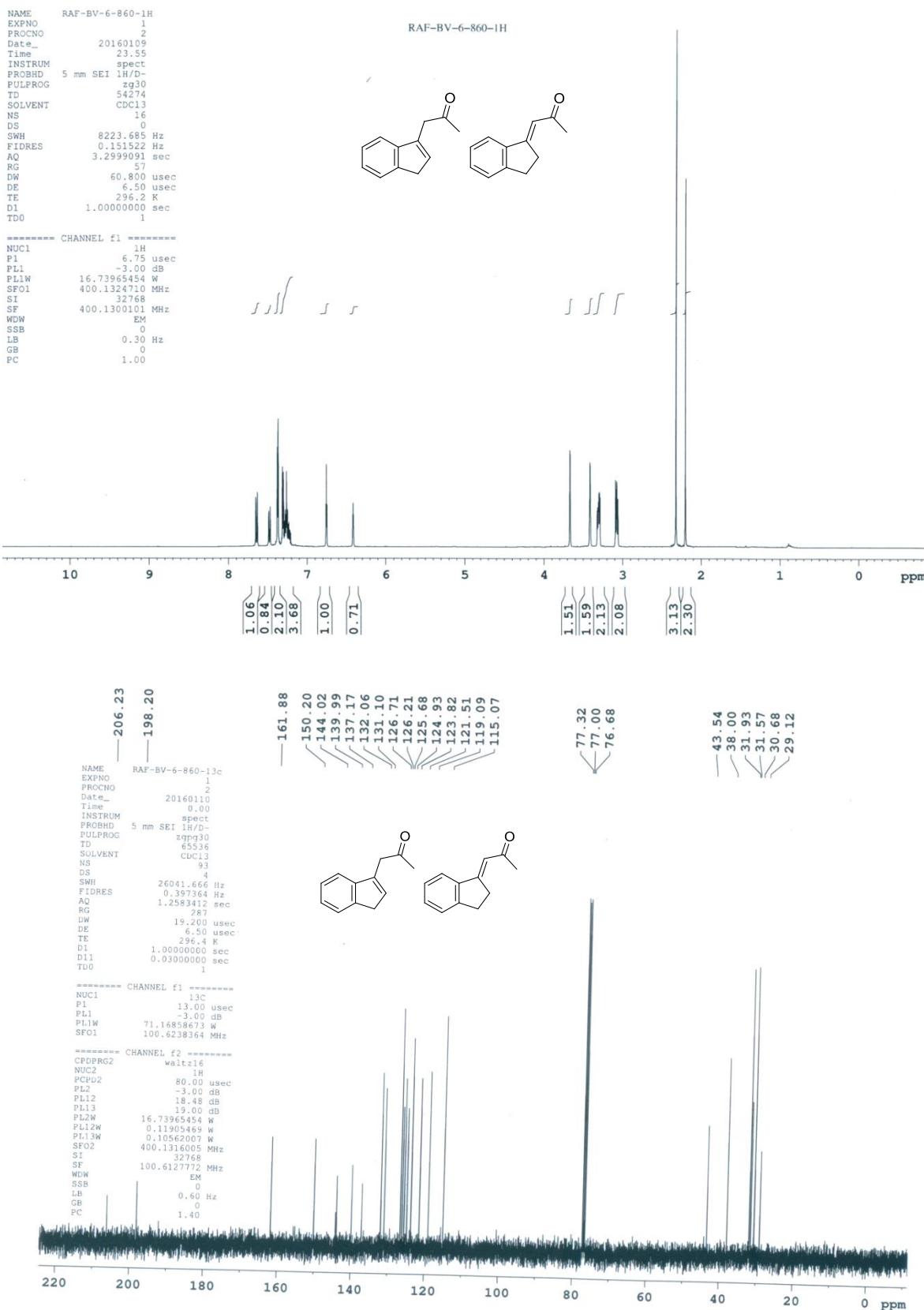
**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 6f**



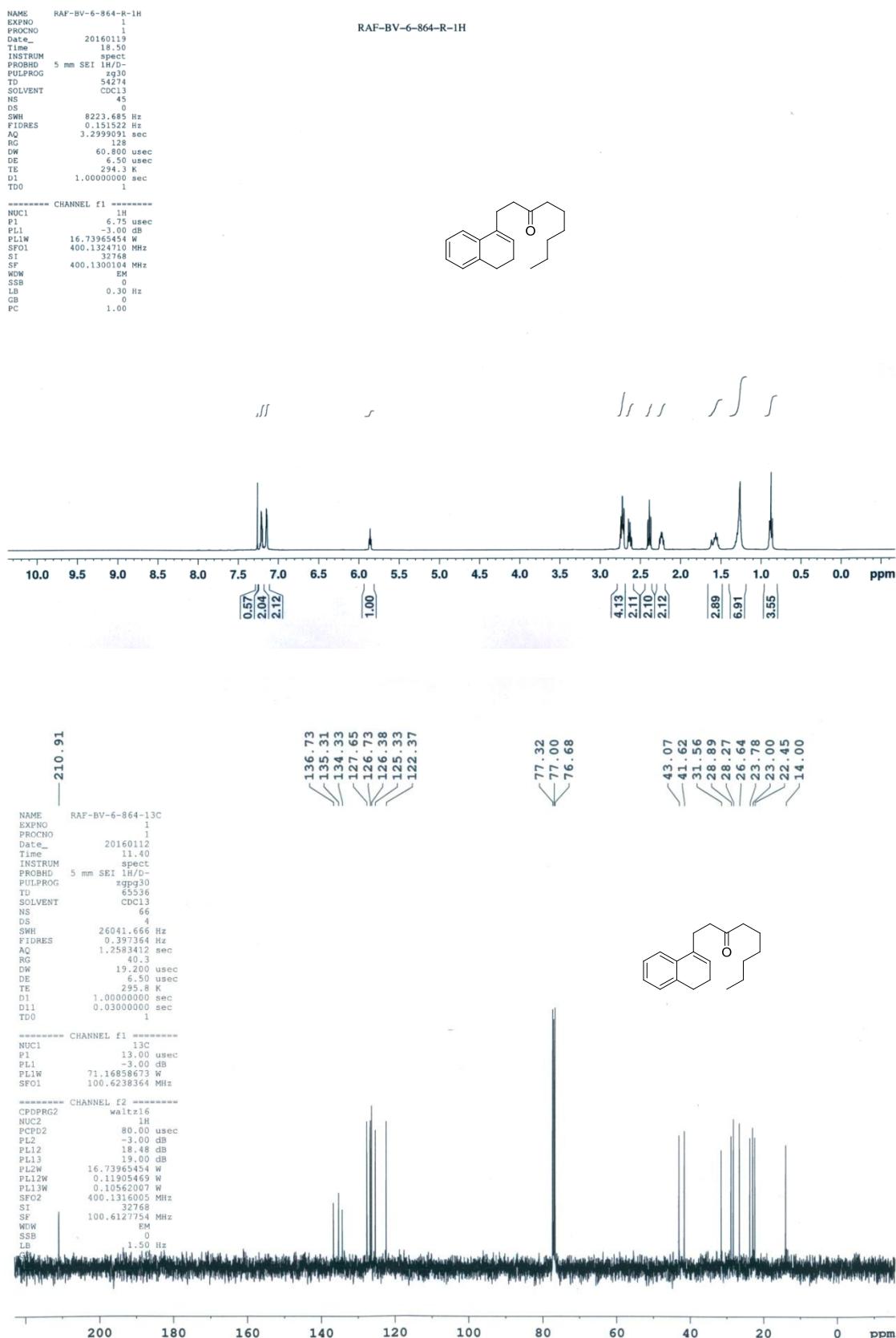
**<sup>1</sup>H NMR (500 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (125 MHz, CDCl<sub>3</sub>) of compound 6g**



**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 6h**



**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 6i**



**<sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>/TMS) and <sup>13</sup>C NMR (100 MHz, CDCl<sub>3</sub>) of compound 6j**

